xrayutilities

version 1.3

Dominik Kriegner

Eugen Wintersberger

April 25, 2016

Contents

Welcome to xrayutilities's documentation!

If you look for downloading the package go to Sourceforge (source distribution) or the Python package index (MS Windows binary). Installation instructions you find further down Installation.

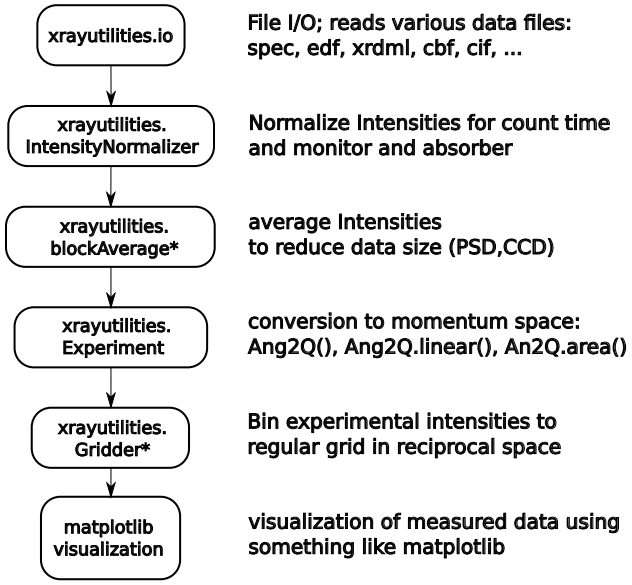
Read more about *xrayutilities* below or in Journal of Applied Crystallography 2013, Volume 46, 1162-1170

Introduction

xrayutilities is a collection of scripts used to analyze and simulate x-ray diffraction data. It consists of a python package and several routines coded in C. It especially useful for the reciprocal space conversion of diffraction data taken with linear and area detectors. Several models for the simulation of thin film reflectivity and diffraction curves are included.

In the following few 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*. Following that the concept of how angular coordinates of Bragg reflections are calculated is presented. Before describing in detail the installation a minimal example for thin film simulations is shown.

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.

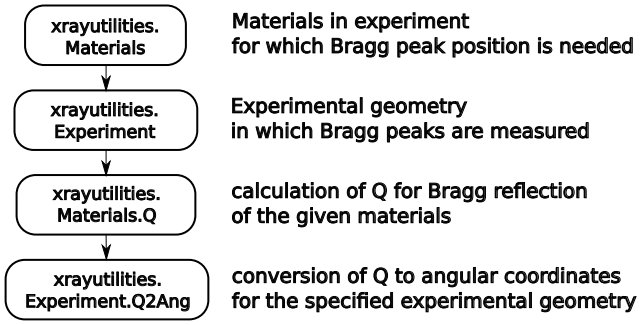
Since the amount of data taken with modern detectors often is too large to be able to work with them properly, a functions for reducing the data from linear and area detectors are provided. They use block-averaging to reduce the amount of data. Use those carefully not to loose the features you are interested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

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, lattice plane distances, 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. In the predefined experimental classes fixed geometries are used. For angle calculation of custom geometries using arbitrary geometries (max. of three free angles) the **`q2ang_fit`**-module can be used as described in one of the included example files.

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
14
15 # global setting for the experiment
16 sample = "test"  # sample name used also as file name for the data file
17 energy = 8042.5  # x-ray energy in eV
18 center_ch = 715.9  # center channel of the linear detector
19 chpdeg = 345.28  # channels per degree of the linear detector
20 roi = [100, 1340]  # region of interest of the detector
21 nchannel = 1500  # number of channels of the detector
22
23 # intensity normalizer function responsible for count time and absorber
24 # correction
25 absfun = lambda d: d["detcorr"] / d["psd2"].astype(numpy.float)
26 normalizer_detcorr = xu.IntensityNormalizer(
27     "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
hxrd = 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
hxrd.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  # try if spec file object already exist ("run -i" in ipython)
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] = hxrd.Q2Ang(
    InP.Q(3, 3, 3))  # nominal values of the substrate peak

# 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.geth5_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] = hxrd.Ang2Q.linear(
    om, tt,
    delta=[omalign - omnominal, ttalign - ttnominal])

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

# plot the intensity as contour plot using matplotlib
plt.figure()
```

```
88 cf = plt.contourf(gridder.xaxis, gridder.yaxis, INT, 100, extend='min')
89 plt.xlabel(r'$Q_{[11\bar2]}$ ($\AA^{-1}$)')
90 plt.ylabel(r'$Q_{[\bar1\bar1\bar1]}$ ($\AA^{-1}$)')
91 cb = plt.colorbar(cf)
92 cb.set_label(r"$\log($Int$)$ (cps)")
```

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

X-ray diffraction and reflectivity simulations

xrayutilties includes a database with optical properties of materials and therefore simulation of reflectivity and diffraction data can be accomplished with relatively litte additional input. When the stack of layers is defined along with the layer thickness and material several models for calculation of X-ray reflectivity and dynamical/kinematical X-ray diffraction are provided.

A minimal example for an AlGaAs superlattice structure is shown below. It shows how a basic stack of a superlattice is built from its ingredients and how the reflectivity and dynamical diffraction model are initialized in the most basic form:

```
import xrayutilities as xu
# Build the pseudomorphic sample stack using the elastic parameters
sub = xu.simpack.Layer(xu.materials.GaAs, inf)
lay1 = xu.simpack.Layer(xu.materials.AlGaAs(0.25), 75, relaxation=0.0)
lay2 = xu.simpack.Layer(xu.materials.AlGaAs(0.75), 25, relaxation=0.0)
pls = xu.simpack.PseudomorphicStack001('pseudo', sub+10*(lay1+lay2))
# simulate reflectivity
m = xu.simpack.SpecularReflectivityModel(pls, sample_width=5, beam_width=0.3)
alphai = linspace(0, 10, 1000)
Ixrr = m.simulate(alphai)
# simulate dynamical diffraction curve
alphai = linspace(29, 38, 1000)
md = xu.simpack.DynamicalModel(pls)
Idyn = md.simulate(alphai, hkl=(0, 0, 4))
```

More detailed examples and description of model parameters can be found on the *Simulation examples* page or in the `examples` directory.

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.

Authors: Dominik Kriegner <dominik.kriegner@gmail.com> and Eugen Wintersberger <eugen.wintersberger@desy.de>

for more details see the full API documentation of **`xrayutilities`** found here: *Examples and API-documentation*.

Installation

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"

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!

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:

- **C-compiler** Gnu Compiler Collection or any compatible C compiler. On windows you most probably want to use the Microsoft compilers.
- **HDF5** a versatile binary data format (library is implemented in C). Although the library is not called directly, it is needed by the h5py Python module (see below).
- **Python** the scripting language in which most of *xrayutilities* code is written in. (version 2.7 or >= 3.2)
- **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 (version >= 1.8)
- **Scipy** a Python module providing standard numerical routines, which is heavily using numpy arrays (version >= 0.11.0)
- **h5py** a powerful Python interface to HDF5.
- **Matplotlib** a Python module for high quality 1D and 2D plotting (optionally)
- **lmfit** a Python module for least-squares minimization with bounds and constraints (optionally needed for fitting XRR data)
- **IPython** although not a dependency of *xrayutilities* the IPython shell is perfectly suited for the interactive use of the *xrayutilities* python package.

For building the documention (which you do not need to do) the requirements are:

- **sphinx** the Python documentation generator
- **numpydoc** sphinx-extension needed to parse the API-documention
- **rst2pdf** pdf-generation using sphinx

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

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 libary is installed under /usr/lib/ on Unix systems or in the Python installation directory on Windows.

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 Python(x,y) 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.

Notes for installing on Windows

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

The setup of the environment variables is also done by the Python distributions. One can proceed with the installation of *xrayutilities* directly! The easiest way to do this on windows is to use the binaries distributed on the Python package index, otherwise one can follow the general installation instructions. Depending on your compiler on Microsoft Windows it might be necessary to perform the building of the Python extension separately and specify the compiler manually. This is done by

```
python setup.py build -c <compiler_name>
```

Using Python(x,y) you want to specify 'mingw32' as compiler name. With the WinPython it is recommended to use the MS Visual Studio Express 2008 (which is freely available for download) and can also build the code for 64bit Windows. In this case us 'msvc' as compiler name.

Examples and API-documentation

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.

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 xrayutilities as xu
 2 import os
 3
 4 # open spec file or use open SPECfile instance
 5 try: s
 6 except NameError:
 7     s = xu.io.SPECFile("sample_name.spec", path="./specdir")
 8
 9 # method (1)
10 s.scan10.ReadData()
11 scan10data = s.scan10.data
12
13 # method (2)
14 h5file = os.path.join("h5dir", "h5file.h5")
15 s.Save2HDF5(h5file) # save content of SPEC file to HDF5 file
16 # read data from HDF5 file
17 [angle1, angle2], scan10data = xu.io.geth5_scan(h5file, [10],
18                                                 "motorname1",
19                                                 "motorname2")
```

Seealso

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 s.scan10.ReadData()
 5 scan10data = s.scan10.data
 6
 7 # reread data method (2)
 8 s.Save2HDF5(h5) # save content of SPEC file to HDF5 file
 9 # read data from HDF5 file
10 [angle1, angle2], scan10data = xu.io.geth5_scan(h5file, [10],
11                                                 "motorname1",
12                                                 "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 if perfectly suited because it can handle large amount of data and compression.:

```
 1 import xrayutilities as xu
 2 import numpy
 3
```

```
specfile = "specfile.spec"
h5file = "h5file.h5"

s = xu.io.SPECFile(specfile)
s.Save2HDF5(h5file) # save to hdf5 file

# read ccd frames from EDF files
for i in range(1, 1001, 1):
    efile = "edfdir/sample_%04d.edf" % i
    e = xu.io.edf.EDFFile(efile)
    e.ReadData()
    e.Save2HDF5(h5file, group="/frelon_%04d" % i)
```

Seealso

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.

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.

```
import xrayutilities as xu
Si = xu.materials.Si  # load material from materials submodule

# initialize experimental class with directions from experiment
hxrd = xu.HXRD(Si.Q(1, 1, -2), Si.Q(1, 1, 1))
# calculate angles of Bragg reflections and print them to the screen
om, chi, phi, tt = hxrd.Q2Ang(Si.Q(1, 1, 1))
print("Si (111)")
print("om,tt: %8.3f %8.3f" % (om, tt))
om, chi, phi, tt = hxrd.Q2Ang(Si.Q(2, 2, 4))
print("Si (224)")
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-alpha1.

One could also call:

```
hxrd = 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 is on implementation of a GID 2S+2D diffractometer. Be sure to check if the order of the detector circles fits your goniometer, otherwise define one yourself!

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-',
20          label="Indium powder convolution")
21 # plot each peak in a bar plot
22 plt.bar(In_powder.ang * 2, In_powder.data / In_powder.data.max(),
23         width=0.3, bottom=0, linewidth=0, color='r',
24         align='center', orientation='vertical', label="Indium bar plot")
25
26 plt.legend(); plt.set_xlim(15, 100); plt.grid()
```

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

```
>>> print In_powder
   Powder diffraction object
   -------------------------
   Material: In
   Lattice:
   a1 = (3.252300 0.000000 0.000000), 3.252300
   a2 = (0.000000 3.252300 0.000000), 3.252300
   a3 = (0.000000 0.000000 4.946100), 4.946100
   alpha = 90.000000, beta = 90.000000, gamma = 90.000000
   Lattice base:
   Base point 0: In (49) (0.000000 0.000000 0.000000) occ=1.00 b=0.00
   Base point 1: In (49) (0.500000 0.500000 0.500000) occ=1.00 b=0.00
   Reflections:
   --------------
         h k l     |    tth    |    |Q|    |    Int     |   Int (%)
      ------------------------------------------------------------
       [-1, 0, -1]    32.9611      2.312       217.75      100.00
        [0, 0, -2]    36.3267      2.541        41.80       19.20
       [-1, -1, 0]    39.1721      2.732        67.72       31.10
```

```
      [-1, -1, -2]    54.4859      3.731        50.75       23.31
      ....
```

Using the `Gridder` classes

xrayutilities provides Gridder classes for 1D, 2D, and 3D data sets. These Gridders map irregular spaced data onto a regular grid. This is often needed after transforming data measured at equally spaced angular positions to reciprocal space were their spacing is irregular.

In 1D this process actually equals the calculation of a histogram. Below you find the most basic way of using the Gridder in 2D. Other dimensions work very similar.

The most easiest use (what most user might need) is:

::

    import xrayutilities as xu # import Python package g = xu.Gridder2D(100, 101) # initialize the Gridder object, which will # perform Gridding to a regular grid with 100x101 points #====== load some data here ===== g(x, y, data) # call the gridder with the data griddata = g.data # the data attribute contains the gridded data.

_.. note: previously you could use the Gridder's gdata object, which was always an internal buffer and should not be used anymore!

A more complicated example showing also sequential gridding is shown below. You need sequential gridding when you can not load all data at the same time, which is often problematic with 3D data sets. In such cases you need to specify the data range before the first call to the gridder.

::

    import xrayutilities as xu # import Python package g = xu.Gridder2D(100, 101) # initialize the Gridder object g.KeepData(True) g.dataRange(1, 2, 3, 4) # (xgrd_min, xgrd_max, ygrd_min, ygrd_max) #====== load some data here ===== g(x, y, data) # call the gridder with the data griddata = g.data # the data attribute contains the so far gridded data.

    #====== load some more data here ===== g(x, y, data) # call the gridder with the new data griddata = g.data # the data attribute contains the combined gridded data.

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
 4 # and lattice constant a
 5 def ZincBlendeLattice(aa, ab, a):
 6     #create lattice base
 7     lb = xu.materials.LatticeBase()
 8     lb.append(aa, [0, 0, 0])
 9     lb.append(aa, [0.5, 0.5, 0])
10     lb.append(aa, [0.5, 0, 0.5])
11     lb.append(aa, [0, 0.5, 0.5])
12     lb.append(ab, [0.25, 0.25, 0.25])
13     lb.append(ab, [0.75, 0.75, 0.25])
14     lb.append(ab, [0.75, 0.25, 0.75])
15     lb.append(ab, [0.25, 0.75, 0.75])
16
17     #create lattice vectors
```

```
18     a1 = [a, 0, 0]
19     a2 = [0, a, 0]
20     a3 = [0, 0, a]
21 
22     l = xu.materials.Lattice(a1, a2, a3, base=lb)
23     return l
24 
25 # defining InP, no elastic properties are given,
26 # helper functions exist to create the (6, 6) elastic tensor
27 # for cubic materials
28 atom_In = xu.materials.elements.In
29 atom_P = xu.materials.elements.P
30 elastictensor = xu.materials.CubicElasticTensor(10.11e+10, 5.61e+10,
31                                                 4.56e+10)
32 InP  = xu.materials.Crystal("InP",
33                             ZincBlendeLattice(atom_In, atom_P, 5.8687),
34                             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)
```

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

Calculation of diffraction angles for a general geometry

Often the restricted predefined geometries are not corresponding to the experimental setup, nevertheless *xrayutilities* is able to calculate the goniometer angles needed to reach a certain reciprocal space position.

For this purpose the goniometer together with the geometric restrictions need to be defined and the q-vector in laboratory reference frame needs to be specified. This works for arbitrary goniometer, however, the user is expected to set up bounds to put restrictions to the number of free angles to obtain reproducible results. In general only three angles are needed to fit an arbitrary q-vector (2 sample + 1 detector angles or 1 sample + 2 detector).

The example below shows the necessary code to perform such an angle calculation for a costum defined material with orthorhombic unit cell.

```
import xrayutilities as xu
import numpy as np

def Pnma(a, b, c):
    #create orthorhombic unit cell
    l = xu.materials.Lattice([a, 0, 0], [0, b, 0], [0, 0, c])
    return l

latticeConstants=[5.600, 7.706, 5.3995]
SmFeO3 = xu.materials.Crystal("SmFeO3", Pnma(*latticeConstants))
# 2S+2D goniometer
qconv=xu.QConversion(('x+', 'z+'), ('z+', 'x+'), (0, 1, 0))
# [1,1,0] surface normal
hxrd = xu.HXRD(SmFeO3.Q(0, 0, 1), SmFeO3.Q(1, 1, 0), qconv=qconv)

hkl=(2, 0, 0)
q_material = SmFeO3.Q(hkl)
q_laboratory = hxrd.Transform(q_material) # transform

print('SmFeO3: \thkl ', hkl, '\tqvec ', np.round(q_material, 5))
print('Lattice plane distance: %.4f' % SmFeO3.planeDistance(hkl))

#### determine the goniometer angles with the correct geometry restrictions
# tell bounds of angles / (min,max) pair or fixed value for all motors
# maximum of three free motors! here incidence angle fixed to 5 degree
# om, phi, tt, delta
bounds = (5, (-180, 180), (-1, 90), (-1, 90))
ang,qerror,errcode = xu.Q2AngFit(q_laboratory, hxrd, bounds)
print('err %d (%.3g) angles %s' % (errcode, qerror, str(np.round(ang, 5))))
# check that qerror is small!!
print('sanity check with back-transformation (hkl): ',
      np.round(hxrd.Ang2HKL(*ang,mat=SmFeO3),5))
```

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 installad 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]
```

```
 3
 4 # verbosity level of information and debugging outputs
 5 #   0: no output
 6 #   1: very import notes for users
 7 #   2: less import notes for users (e.g. intermediate results)
 8 #   3: debuging output (e.g. print everything, which could be interesing)
 9 #   levels can be changed in the config file as well
10 verbosity = 1
11
12 # default wavelength in Angstrom,
13 wavelength = MoKa1 # Molybdenum K alpha1 radiation (17479.374eV)
14
15 # default energy in eV
16 # if energy is given wavelength settings will be ignored
17 #energy = 10000 #eV
18
19 # number of threads to use in parallel sections of the code
20 nthreads = 1
21 #   0: the maximum number of available threads will be used (as returned by
22 #      omp_get_max_threads())
23 #   n: n-threads will be used
```

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,
23                                                       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
 3 from images recorded in the primary beam
 4 """
 5
 6 import xrayutilities as xu
 7 import os
 8
 9 en = 10300.0  # eV
10 datadir = os.path.join("data", "wire_")  # data path for CCD files
11 # template for the CCD file names
12 filetmp = os.path.join(datadir, "wire_12_%05d.edf.gz")
13
14 # manually selected images
15 # select images which have the primary beam fully on the CCD
16 imagenrs = [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19,
17             20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33]
18
19 images = []
20 ang1 = []
21 ang2 = []
22
23 # read images and angular positions from the data file
24 # this might differ for data taken at different beamlines since
25 # they way how motor positions are stored is not always consistent
26 for imgnr in imagenrs:
27     filename = filetmp % imgnr
28     edf = xu.io.EDFFile(filename)
29     images.append(edf.data)
30     ang1.append(float(edf.header['ESRF_ID01_PSIC_NANO_NU']))
31     ang2.append(float(edf.header['ESRF_ID01_PSIC_NANO_DEL']))
32
33
34 # call the fit for the detector parameters
35 # detector arm rotations and primary beam direction need to be given.
```

```
# in total 8 parameters are fitted, however the 4 misalignment parameters can
# be fixed they are the detector tilt azimuth, the detector tilt angle, the
# detector rotation around the primary beam and the outer angle offset
param, eps = xu.analysis.sample_align.area_detector_calib(
    ang1, ang2, images, ['z+', 'y-'], 'x+', start=(45, 0, -0.7, 0),
    fix=(False, False, False, False), wl=xu.en2lam(en))
```

A possible output of this script could be

> fitted parameters: epsilon: 8.0712e-08 (2,['Parameter convergence']) param: (cch1,cch2,pwidth1,pwidth2,tiltazimuth,tilt,detrot,outerangle_offset) param: 140.07 998.34 4.4545e-05 4.4996e-05 72.0 1.97 -0.792 -1.543 please check the resulting data (consider setting plot=True) detector rotation axis / primary beam direction (given by user): ['z+', 'y-'] / x+ detector pixel directions / distance: z- y+ / 1 detector initialization with: init_area('z-', 'y+', cch1=140.07, cch2=998.34, Nch1=516, Nch2=516, pwidth1=4.4545e-05, pwidth2=4.4996e-05, distance=1., detrot=-0.792, tiltazimuth=72.0, tilt=1.543) AND ALWAYS USE an (additional) OFFSET of -1.9741deg in the OUTER DETECTOR ANGLE!

The output gives the fitted detector parameters and compiles the Python code line one needs to use to initialize the detector. Important to note is that the outer angle offset which was determined by the fit (-1.9741 degree in the aboves example) is not included in the initialization of the detector parameters *but* needs to be used in every call to the q-conversion function as offset. This step needs to be performed manually by the user!

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

```
"""
example script to show the detector parameter determination for area detectors
from images recorded in the primary beam and at known symmetric coplanar Bragg
reflections of a reference crystal
"""

import xrayutilities as xu
import os
import numpy

Si = xu.materials.Si

datadir = 'data'
specfile = "si_align.spec"

en = 15000  # eV
wl = xu.en2lam(en)
imgdir = os.path.join(datadir, "si_align_")  # data path for CCD files
filetmp = "si_align_12_%04d.edf.gz"

qconv = xu.QConversion(['z+', 'y-'], ['z+', 'y-'], [1, 0, 0])
hxrd = xu.HXRD(Si.Q(1, 1, -2), Si.Q(1, 1, 1), wl=wl, qconv=qconv)

# manually selected images

s = xu.io.SPECFile(specfile, path=datadir)
```

```
for num in [61, 62, 63, 20, 21, 26, 27, 28]:
    s[num].ReadData()
    try:
        imagenrs = numpy.append(imagenrs, s[num].data['ccd_n'])
    except:
        imagenrs = s[num].data['ccd_n']

# avoid images which do not have to full beam on the detector as well as
# other which show signal due to cosmic radiation
avoid_images = [37, 57, 62, 63, 65, 87, 99, 106, 110, 111, 126, 130, 175,
                181, 183, 185, 204, 206, 207, 208, 211, 212, 233, 237, 261,
                275, 290]

images = []
ang1 = []  # outer detector angle
ang2 = []  # inner detector angle
sang = []  # sample rocking angle
hkls = []  # Miller indices of the reference reflections


def hotpixelkill(ccd):
    """
    function to remove hot pixels from CCD frames
    ADD REMOVE VALUES IF NEEDED!
    """
    ccd[304, 97] = 0
    ccd[303, 96] = 0
    return ccd

# read images and angular positions from the data file
# this might differ for data taken at different beamlines since
# they way how motor positions are stored is not always consistent
for imgnr in numpy.sort(list(set(imagenrs) - set(avoid_images))[::4]):
    filename = os.path.join(imgdir, filetmp % imgnr)
    edf = xu.io.EDFFile(filename)
    ccd = hotpixelkill(edf.data)
    images.append(ccd)
    ang1.append(float(edf.header['motor_pos'].split()[4]))
    ang2.append(float(edf.header['motor_pos'].split()[3]))
    sang.append(float(edf.header['motor_pos'].split()[1]))
    if imgnr > 1293.:
        hkls.append((0, 0, 0))
    elif imgnr < 139:
        hkls.append((0, 0, numpy.sqrt(27)))  # (3,3,3))
    else:
        hkls.append((0, 0, numpy.sqrt(75)))  # (5,5,5))

# call the fit for the detector parameters.
# Detector arm rotations and primary beam direction need to be given
# in total 8 detector parameters + 2 additional parameters for the reference
# crystal orientation and the wavelength are fitted, however the 4 misalignment
# parameters of the detector and the 3 other parameters can be fixed.
# The fixable parameters are detector tilt azimuth, the detector tilt angle,
# the detector rotation around the primary beam, the outer angle offset, sample
# tilt, sample tilt azimuth and the x-ray wavelength
param, eps = xu.analysis.area_detector_calib_hkl(
    sang, ang1, ang2, images, hkls, hxrd, Si, ['z+', 'y-'], 'x+',
    start=(45, 1.69, -0.55, -1.0, 1.3, 60., wl),
    fix=(False, False, False, False, False, False, False),
    plot=True)
```

```
 87
 88 # Following is an example of the output of the summary of the
 89 # area_detector_calib_hkl function
 90 # total time needed for fit: 624.51sec
 91 # fitted parameters: epsilon: 9.9159e-08 (2,['Parameter convergence'])
 92 # param:
 93 # (cch1,cch2,pwidth1,pwidth2,tiltazimuth,tilt,detrot,outerangle_offset,
 94 # sampletilt,stazimuth,wavelength)
 95 # param: 367.12 349.27 6.8187e-05 6.8405e-05 131.4 2.87 -0.390 -0.061 1.201
 96 # 318.44 0.8254
 97 # please check the resulting data (consider setting plot=True)
 98 # detector rotation axis / primary beam direction (given by user): ['z+', 'y-']
 99 # / x+
100 # detector pixel directions / distance: z- y+ / 1
101 #   detector initialization with:
102 #   init_area('z-', 'y+', cch1=367.12, cch2=349.27, Nch1=516, Nch2=516,
103 #   pwidth1=6.8187e-05, pwidth2=6.8405e-05, distance=1., detrot=-0.390,
104 #   tiltazimuth=131.4, tilt=2.867)
105 # AND ALWAYS USE an (additional) OFFSET of -0.0611deg in the OUTER
106 # DETECTOR ANGLE!
```

Simulation examples

In the following a few code-snippets are shown which should help you getting started with reflectivity and diffraction simulations using *xrayutilities*. All simulations in *xrayutilities* are for layers systems and currently there are no plans to extend this to other geometries. Note that not all of the codes shown in the following will be run-able as stand-alone scripts. For fully running scripts look in the `examples` directory in the download found here.

Building Layer stacks for simulations

The basis of all simulations in *xrayutilities* are stacks of layers. Therefore several functions exist to build up such layered systems. The basic building block of all of them is a **`Layer`** object which takes a material and its thickness in ångström as initializing parameter.:

```
import xrayutilities as xu
lay = xu.simpack.Layer(xu.materials.Si, 200)
```

In the shown example a silicon layer with 20 nm thickness is created. The first argument is the material of the layer. For diffraction simulations this needs to be derived from the **`Crystal`**-class. This means all predefined materials in *xrayutitities* can be used for this purpose. For x-ray reflectivity simulations, however, also knowing the chemical composition and density of the material is sufficient.

A 5 nm thick metallic CoFe compound layer can therefore be defined by:

```
rho_cf = 0.5*8900 + 0.5*7874  # mass density in kg/m^3
mCoFe = xu.materials.Amorphous('CoFe', rho_cf, [('Co', 0.5), ('Fe', 0.5)])
lCoFe = xu.simpack.Layer(mat_cf, 50)
```

Note

The **`Layer`** object can have several more model dependent properties discussed in detail below.

When several layers are defined they can be combined to a **`LayerStack`** which is used for the simulations below.:

```
1 sub = xu.simpack.Layer(xu.materials.Si, inf)
2 lay1 = xu.simpack.Layer(xu.materials.Ge, 200)
3 lay2 = xu.simpack.Layer(xu.materials.SiO2, 30)
4 ls = xu.simpack.LayerStack('Si/Ge', sub, lay1, lay2)
```

```
5 # or equivalently
6 ls = xu.simpack.LayerStack('Si/Ge', sub + lay1 + lay2)
```

The last two lines show two different options of creating a stack of layers. As is shown in the last example the substrate thickness can be infinite (see below) and layers can be also stacked by summation. For creation of more complicated superlattice stacks one can further use multiplication:

```
lay1 = xu.simpack.Layer(xu.materials.SiGe(0.3), 50)
lay2 = xu.simpack.Layer(xu.materials.SiGe(0.6), 40)
ls = xu.simpack.LayerStack('Si/SiGe SL', sub + 5*(lay1 + lay2))
```

Pseudomorphic Layers

All stacks of layers described above use the materials in the layer as they are supplied. However, epitaxial systems often adopt the inplane lattice parameter of the layers beneath. To mimic this behavior you can either supply the **`Layer`** objects which custom **`Crystal`** objects which have the appropriate lattice parameters or use the **`PseudomorphicStack*`** classes which to the adaption of the lattice parameters automatically. In this respect the 'relaxation' parameter of the **`Layer`** class is important since it allows to create partially/fully relaxed layers.:

```
1 sub = xu.simpack.Layer(xu.materials.Si, inf)
2 buf1 = xu.simpack.Layer(xu.materials.SiGe(0.5), 5000, relaxation=1.0)
3 buf2 = xu.simpack.Layer(xu.materials.SiGe(0.8), 5000, relaxation=1.0)
4 lay1 = xu.simpack.Layer(xu.materials.SiGe(0.6), 50, relaxation=0.0)
5 lay2 = xu.simpack.Layer(xu.materials.SiGe(1.0), 50, relaxation=0.0)
6 # create pseudomorphic superlattice stack
7 pls = xu.simpack.PseudomorphicStack001('SL 5/5', sub+buf1+buf2+5*(lay1+lay2))
```

Note

As indicated by the function name the PseudomorphicStack currently only works for (001) surfaces and cubic materials. Implementations for other surface orientations are planned.

If you would like to check the resulting lattice objects of the different layers you could use:

```
for l in pls:
    print(l.material.lattice)
```

Special layer types

So far one special layer mimicking a layer with gradually changing chemical composition is implemented. It consists of several thin sublayers of constant composition. So in order to obtain a smooth grading one has to select enough sublayers. This however has a negativ impact on the performance of all simulation models. A tradeoff needs to found! Below a graded SiGe buffer is shown which consists of 100 sublayers and has total thickness of 1µm.:

```
1 buf = xu.simpack.GradedLayerStack(xu.materials.SiGe,
2                                   0.2,  # xfrom Si0.8Ge0.2
3                                   0.7,  # xto Si0.3Ge0.7
4                                   100,  # number of sublayers
5                                   10000,  # total thickness
6                                   relaxation=1.0)
```

Setting up a model

This sectiondescribes the parameters which are common for all diffraction models in *xrayutilties*-`simpack`. All models need a list of Layers for which the reflected/diffracted signal will be calculated. Further all models have some common parameters which allow scaling and background addition in the model output and contain general information about the calculation which are model-independent. These are

- 'experiment': an **Experiment**/**HXRD** object which defines the surface geometry of the model. If none is given a default class with (001) surface is generated.
- 'resolution_width': width of the Gaussian resolution function used to convolute with the data. The unit of this parameters depends on the model and can be either in degree or 1/AA.
- 'I0': is the primary beam flux/intensity
- 'background': is the background added to the simulation after it was scaled by I0
- 'energy': energy in eV used to obtain the optical parameters for the simulation. The energy can alternatively also be supplied via the 'experiment' parameter, however, the 'energy' value overrules this setting. If no energy is given the default energy from the configuration is used.

The mentioned parameters can be supplied to the constructor method of all model classes derived from **LayerModel**, which applies to all examples mentioned below.:

```
m = xu.simpack.SpecularReflectivityModel(layerstack, I0=1e6, background=1,
                                         resolution_width=0.001)
```

Reflectivity calculation and fitting

Currently only the Parrat formalism including non-correlated roughnesses is included for specular x-ray reflectivity calculations. A minimal working example for a reflectivity calculation follows.:

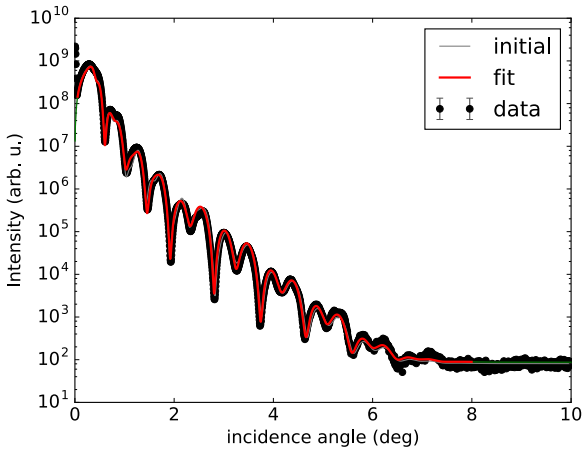
```
 1 # building a stack of layers
 2 sub = xu.simpack.Layer(xu.materials.GaAs, inf, roughness=2.0)
 3 lay1 = xu.simpack.Layer(xu.materials.AlGaAs(0.25), 75, roughness=2.5)
 4 lay2 = xu.simpack.Layer(xu.materials.AlGaAs(0.75), 25, roughness=3.0)
 5 pls = xu.simpack.PseudomorphicStack001('pseudo', sub+5*(lay1+lay2))
 6
 7 # reflectivity calculation
 8 m = xu.simpack.SpecularReflectivityModel(pls, sample_width=5, beam_width=0.3)
 9 ai = linspace(0, 5, 10000)
10 Ixrr = m.simulate(ai)
```

In addition to the layer thickness also the roughness and relative density of a Layer can be set since they are important for the reflectivity calculation. This can be done upon definition of the **Layer** or also manipulated at any later stage. Such x-ray reflectivity calculations can also be fitted to experimental data using the **fit_xrr()** function which is shown in detail in the example below (which is also included in the example directory). The fitting is performed using the lmfit Python package which needs to be installed when you want to use this fitting function. This package allows to build complicated models including bounds and correlations between parameters.

```
 1 from matplotlib.pylab import *
 2 import xrayutilities as xu
 3 import lmfit
 4 import numpy
 5
 6 # load experimental data
 7 ai, edata, eps = numpy.loadtxt('data/xrr_data.txt'), unpack=True)
 8 ai /= 2.0
 9
10 # define layers
11 # SiO2 / Ru(5) / CoFe(3) / IrMn(3) / AlOx(10)
12 lSiO2 = xu.simpack.Layer(xu.materials.SiO2, inf)
13 lRu = xu.simpack.Layer(xu.materials.Ru, 50)
14 rho_cf = 0.5*8900 + 0.5*7874
15 mat_cf = xu.materials.Amorphous('CoFe', rho_cf, [('Co', 0.5), ('Fe', 0.5)])
16 lCoFe = xu.simpack.Layer(mat_cf, 30)
17 lIrMn = xu.simpack.Layer(xu.materials.Ir20Mn80, 30)
18 lAl2O3 = xu.simpack.Layer(xu.materials.Al2O3, 100)
19
20 m = xu.simpack.SpecularReflectivityModel(lSiO2, lRu, lCoFe, lIrMn, lAl2O3,
21                                          energy='CuKa1')
```

```
22
23 p = lmfit.Parameters()
24 #          (Name                ,     Value,  Vary,    Min,  Max, Expr)
25 p.add_many(('SiO2_thickness'     , numpy.inf, False,  None, None, None),
26            ('SiO2_roughness'     ,       2.5,  True,     0,    8, None),
27            ('Ru_thickness'       ,      47.0,  True,    25,   70, None),
28            ('Ru_roughness'       ,       2.8,  True,     0,    8, None),
29            ('Ru_density'         ,       1.0,  True,   0.8,  1.0, None),
30            ('CoFe_thickness'     ,      27.0,  True,    15,   50, None),
31            ('CoFe_roughness'     ,       4.6,  True,     0,    8, None),
32            ('CoFe_density'       ,       1.0,  True,   0.8,  1.2, None),
33            ('Ir20Mn80_thickness',      21.0,  True,    15,   40, None),
34            ('Ir20Mn80_roughness',       3.0,  True,     0,    8, None),
35            ('Ir20Mn80_density'   ,       1.1,  True,   0.8,  1.2, None),
36            ('Al2O3_thickness'    ,     100.0,  True,    70,  130, None),
37            ('Al2O3_roughness'    ,       5.5,  True,     0,    8, None),
38            ('Al2O3_density'      ,       1.0,  True,   0.8,  1.2, None),
39            ('I0'                 ,    6.75e9,  True,   3e9,  8e9, None),
40            ('background'         ,        81,  True,    40,  100, None),
41            ('sample_width'       ,       6.0, False,     2,    8, None),
42            ('beam_width'         ,      0.25, False,   0.2,  0.4, None),
43            ('resolution_width'   ,      0.02, False,  0.01, 0.05, None))
44
45 res = xu.simpack.fit_xrr(m, p, ai, data=edata, eps=eps, xmin=0.05, xmax=8.0,
46                          plot=True, verbose=True)
47 lmfit.report_fit(res, min_correl=0.5)
```

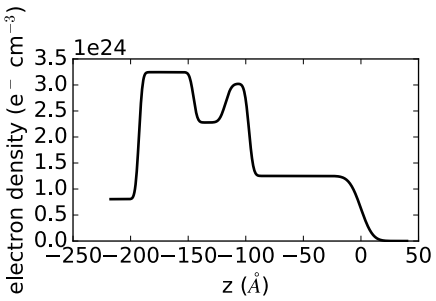
This script can interactively show the fitting progress and after the fitting shows the final plot including the x-ray reflectivity trace of the initial and final parameters.



The picture shows the final plot of the fitting example shown in one of the example scripts.

After building a `SpecularReflectivityModel` is built or fitted the density profile resulting from the thickness and roughness of layers can be plotted easily by:

```
m.densityprofile(500, plot=True)  # 500 number of points
```



Diffraction calculation

From the very same models as used for XRR calculation one can also perform crystal truncation rod simulations around certain Bragg peaks using various different diffraction models. Depending on the system to model you will have to choose the most apropriate model. Below a short description of the implemented models is given followed by two examples.

Kinematical diffraction models

The most basic models consider only the kinematic diffraction of layers and substrate. Especially the semiinfinite substrate is not well described using the kinematical approximation which results in considerable deviations in close vicinity to substrate Bragg peak with respect to the more acurate dynamical diffraction models.

Such a basic model is employed by:

```
mk = xu.simpack.KinematicalModel(pls, energy=en, resolution_width=0.0001)
Ikin = mk.simulate(qz, hkl=(0, 0, 4))
```

A more appealing kinematical model is represented by the `KinematicalMultiBeamModel` class which implements a true multibeam theory is, however, restricted to the use of (001) surfaces and layer thicknesses will be changed to be a multiple of the out of plane lattice spacing. This is necessary since otherwise the structure factor of the unit cell can not be used for the calculation.

It can be employed by:

```
mk = xu.simpack.KinematicalMultiBeamModel(pls, energy=en,
                                          surface_hkl=(0, 0, 1),
                                          resolution_width=0.0001)
Imult = mk.simulate(qz, hkl=(0, 0, 4))
```

This model is expected to provide good results especially far away from the substrate peak where the influence of other Bragg peaks on the truncation rod and the variation of the structure factor can not be neglected.

Both kinematical model's `simulate()` method offers two keyword arguments with which basic absorption and refraction correction can be added to the basic models.

Note

The kinematical models can also handle a semi-infinitely thick substrate which results in a diverging intensity at the Bragg peak but provides a basic description of the substrates truncation rod.

Dynamical diffraction models

Acurate description of the diffraction from thin films in close vicinity to the diffraction signal from a bulk substrate is only possible using the dynamical diffraction theory. In **xrayutilities** the dynamical two-beam theory with 4 tiepoints for the calculation of the dispersion surface is implemented. To use this theory you have to supply the `simulate()` method with the incidence angle in degree. Accordingly the 'resolution_width' parameter is also in degree for this model.:

```
md = xu.simpack.DynamicalModel(pls, energy=en, resolution_width=resol)
Idyn = md.simulate(ai, hkl=(0, 0, 4))
```

A second simplified dynamical model (**`SimpleDynamicalCoplanarModel`**) is also implemented should, however, not be used since its approximations cause mistakes in almost all relevant cases.

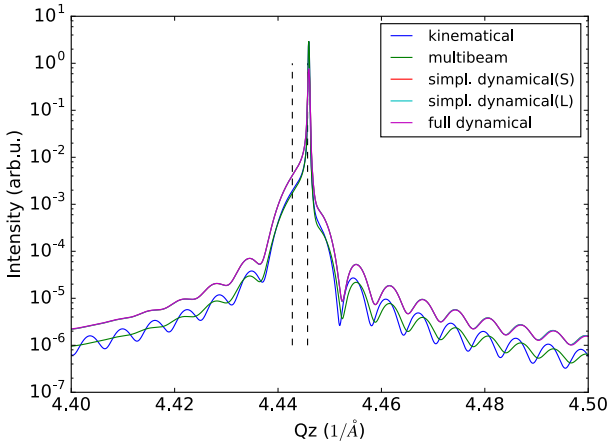
The **`DynamicalModel`** supports the calculation of diffracted signal for 'S' and 'P' polarization geometry. To simulate diffraction data of laboratory sources with Ge(220) monochromator crystal one should use:

```
1 qGe220 = linalg.norm(xu.materials.Ge.Q(2, 2, 0))
2 thMono = arcsin(qGe220 * lam / (4*pi))
3 md = xu.simpack.DynamicalModel(pls, energy='CuKa1',
4                                 Cmono=cos(2 * thMono),
5                                 polarization='both')
6 Idyn = md.simulate(ai, hkl=(0, 0, 4))
```

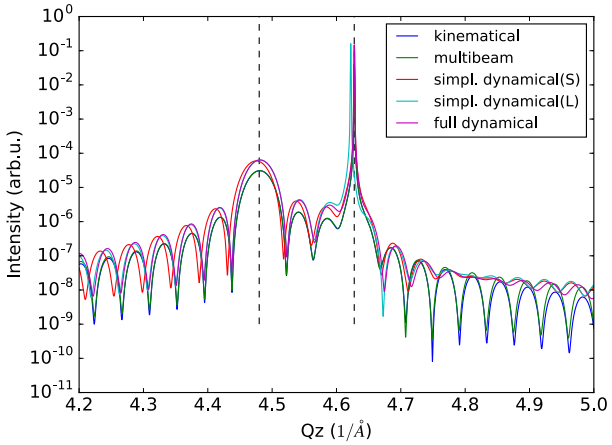
Comparison of diffraction models

Below we show the different implemented models for the case of epitaxial GaAs/AlGaAs and Si/SiGe bilayers. These two cases have very different separation of the layer Bragg peak from the substrate and therefore provide good model system for our models.

We will compare the (004) Bragg peak calculated with different models and but otherwise equal parameters. For scripts used to perform the shown calculation you are referred to the `examples` directory.



XRD simulations of the (004) Bragg peak of ~100 nm AlGaAs on GaAs(001) using various diffraction models



XRD simulations of the (004) Bragg peak of 15 nm $Si_{0.4}Ge_{0.6}$ on Si(001) using various diffraction models

As can be seen in the images we find that for the AlGaAs system all models except the very basic kinematical model yield an very similar diffraction signal. The second kinematic diffraction model considering the contribution of multiple

Bragg peaks on the same truncation rod fails to describe only the ratio of substrate and layer signal, but otherwise results in a very similar line shape as the traces obtained by the dynamic theory.

For the SiGe/Si bilayer system bigger differences between the kinematic and dynamic models are found. Further also the difference between the simpler and more sophisticated dynamic model gets obvious further away from the reference position. Interestingly also the multibeam kinematic theory differs considerable from the best dynamic model. As is evident from this second comparison the correct choice of model for the particular system under condideration is crucial for comparison with experimental data.

xrayutilities package

Subpackages

xrayutilities.analysis package

Submodules

xrayutilities.analysis.line_cuts module

`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 extraced scan (bounds=True)

Examples

```
>>> 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`*, *`ttcenter`*, *`omrange`*, *`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

Examples

```
>>> 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 extraced scan (bounds=True)

Examples

```
>>> 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

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)
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

Examples

```
>>> 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

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)

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

Examples

```
>>> 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

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)

qxpos: position at which the line scan should be extracted

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

angrange: integration range in angular 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)

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

wl: wavelength used to determine angular integration positions

Returns

qz,qzint: qz scan coordinates and intensities (bounds=False)

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

Examples

```
>>> 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

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: om-position at which the radial scan should be extracted

ttcenter: tt-position at which the radial scan should be extracted

ttrange: two theta range of the radial scan to extract

npoints: number of points of the radial scan

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

omrange: 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 two theta positions are returned (default=True)

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

Returns

om,tt,radint: omega,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)

Examples

```
>>> 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

omcenter: om-position at which the radial scan should be extracted

ttcenter: tt-position at which the radial scan should be extracted

ttrange: two theta range of the radial scan to extract

npoints: number of points of the radial scan

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

omrange: integration range perpendicular to scan direction

lam: wavelength for use in the conversion to angular coordinates

Returns

qxrad,qzrad: reciprocal space boundaries of radial scan

Examples

```
>>>
```

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

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 radial scan should be extracted
qzcenter: qz-position at which the radial scan should be extracted
ttrange: two theta range of the radial scan to extract
npoints: number of points of the radial scan

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

omrange: 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

om,tt,radint: omega,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)

Examples

```
>>> 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

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: om-position at which the 2theta scan should be extracted
ttcenter: tt-position at which the 2theta scan should be extracted
ttrange: two theta range of the scan to extract
npoints: number of points of the radial scan

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

omrange: integration range in omega 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint: two 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)

Examples

```
>>> 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

omcenter:	om-position at which the 2theta scan should be extracted
ttcenter:	tt-position at which the 2theta scan should be extracted
ttrange:	two theta range of the 2theta scan to extract
npoints:	number of points of the 2theta scan

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

omrange:	integration range in omega direction
lam:	wavelength for use in the conversion to angular coordinates

Returns

qxtt,qztt:	reciprocal 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)

Examples

```
>>>
```

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

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 2theta scan should be extracted
qzcenter:	qz-position at which the 2theta scan should be extracted
ttrange:	two theta range of the scan to extract
npoints:	number of points of the radial scan

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

omrange:	integration range in omega 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 two theta positions are returned (default=True)
bounds:	flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint:	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)

Examples

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

xrayutilities.analysis.line_cuts.**getindex** (*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,y:	coordinates of the point of interest (float)
xgrid,ygrid:	grid coordinates in x and y direction (array)

Returns

ix,iy: index of the closest gridpoint (lower left) of the point (x,y)

xrayutilities.analysis.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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

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

xrayutilities.analysis.line_cuts3d.**getindex3d** (*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)

xrayutilities.analysis.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
Parameters

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

Examples

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])

xrayutilities.analysis.sample_align module

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

xrayutilities.analysis.sample_align.**area_detector_calib** (*angle1*, *angle2*, *ccdimages*, *detaxis*, *r_i*, *plot=True*, *cut_off=0.7*, *start=(0*, *0*, *0*, *0)*, *fix=(False*, *False*, *False*, *False)*, *fig=None*, *wl=None*, *plotlog=False*, *nwindow=50*, *debug=False*)
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
angle2: inner detector arm angle
ccdimages: images of the ccd taken at the angles given above
detaxis: detector arm rotation axis :default: ['z+','y-']
r_i: primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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. By default (0,0,0,0) is used.
- **fix:** fix parameters of start (default: (False,False,False,False))
- **fig:** matplotlib figure used for plotting the error :default: None (creates own figure)
- **wl:** wavelength of the experiment in Angstrom (default: config.WAVELENGTH) value does not really matter here but does affect the scaling of the error
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to specify that you want to see verbose output and saving of images to show if the CEN determination works

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*, *False)*, *fig=None*, *plotlog=False*, *nwindow=50*, *debug=False*)

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. Both images from the primary beam hkl = (0,0,0) and from a symmetric reflection hkl = (h,k,l) need to be given for a successful run.

parameters

- **sampleang:** sample 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
- **angle1:** outer detector arm angle
- **angle2:** inner detector arm angle
- **ccdimages:** images of the ccd taken at the angles given above
- **hkls:** array/list of hkl values for every image
- **experiment:** Experiment class object needed to get the UB matrix for the hkl peak treatment
- **material:** material used as reference crystal
- **detaxis:** detector arm rotation axis :default: ['z+','y-']
- **r_i:** primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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: 0.1 = 10%
- **start:** sequence of start values of the fit for parameters, which can not be estimated automatically. these are: tiltazimuth, tilt, detector_rotation, outerangle_offset, sampletilt, sampletiltazimuth, 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))
- **fig:** matplotlib figure used for plotting the error. :default: None (creates own figure)
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to tell if you want to see debug output of the script (switch this to true only if you can handle it :))

xrayutilities.analysis.sample_align.**fit_bragg_peak** (*om*, *tt*, *psd*, *omalign*, *ttalign*, *exphxrd*, *frange=(0.03*, *0.03)*, *peaktype='Gauss'*, *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) or Lorentzian (xrayutilities.math.Lorentz2d)
PLEASE ALWAYS CHECK THE RESULT CAREFULLY!
Parameters

- **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 +/-frangeAA^{-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})
- **peaktype:** can be 'Gauss' or 'Lorentz' to fit either of the two peak shapes
- **plot:** if True (default) function will plot the result of the fit in comparison with the measurement.

Returns

- **Omfit,ttfit,paramss,covariance:** fitted angular values, and the fit parameters (of the Gaussian/Lorentzian) 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)

keyword arguments:

- **r_i:** primary beam direction as vector [xyz][+-]; default: 'y+'
- **detaxis:** detector arm rotation axis [xyz][+-]; default: 'x+'

other options are passed to psd_chdeg function, options include:

plot: flag to specify if a visualization of the fit should be done

usetilt: whether to use model considering a detector tilt, i.e. 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/pixelwidth*pi/180 ~= 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*, *omega0=None*, *plot=True*)

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

phi: azimuths 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.

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.

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

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'*, *mtiltlabel='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*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, i.e. deviation angle of the pixel direction from orthogonal to the primary beam :(default: True)

datap: plot format of data points

modelline: plot format of modelline

modeltilt: plot format of modeltilt

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/pixelwidth*pi/180 = channel/degree for large detector distance with the sample detector disctance 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

Examples

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

Module contents

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.

xrayutilities.io package

Submodules

xrayutilities.io.cbf module

class xrayutilities.io.cbf.**CBFDirectory** (*datapath*, *ext='cbf'*, ***keyargs*)
Bases: **object**
Parses a directory for CBF files, which can be stored to a HDF5 file for further usage

Save2HDF5 (*h5f*, *group=''*, *comp=True*)
Saves the data stored in the CBF 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.
Parameters

h5f: a HDF5 file object or name

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.cbf.**CBFFile** (*fname*, *nxkey='X-Binary-Size-Fastest-Dimension'*, *nykey='X-Binary-Size-Second-Dimension'*, *dtkey='DataType'*, *path=None*)
Bases: **object**

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

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

xrayutilities.io.cbf.**makeNaturalName** (*name*)

xrayutilities.io.desy_tty08 module

class for reading data + header information from tty08 data files

tty08 is a system used at beamline P08 at Hasylab Hamburg and creates simple ASCII files to save the data. Information is easily read from the multicolumn data file. the functions below enable also to parse the information of the header

xrayutilities.io.desy_tty08.**gettty08_scan** (*scanname*, *scannumbers*, **args*, ***keyargs*)
function to obtain the angular cooridinates as well as intensity values saved in TTY08 datafiles. Especially usefull for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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)

**keyargs: keyword arguments are passed on to tty08File
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']).

Examples

```
>>> [om,tt],MAP = xu.io.gettty08_scan('text%05d.dat',36,'omega','gamma')
```

class xrayutilities.io.desy_tty08.**tty08File** (*filename*, *path=None*, *mcadir=None*)

Bases: **object**

Represents a tty08 data file. The file is read during the Constructor call. This class should work for data stored at beamline P08 using the tty08 acquisition system.

Required constructor arguments:

filename: a string with the name of the tty08-file

Optional keyword arguments:

mcadir: directory name of MCA files

Read ()

Read the data from the file

ReadMCA ()

xrayutilities.io.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 (*h5f*, *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.

Parameters

h5f: a HDF5 file object or name

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*, *keep_open=False*)

Bases: **object**

Parse ()

Parse file to find the number of entries and read the respective header information

ReadData (*nimg=0*)

Read the CCD data of the specified image and return the data this function is called automatically when the 'data' property is accessed, but can also be called manually when only a certain image from the file is needed.

Parameters

nimg: number of the image which should be read (starts with 0)

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

data

xrayutilities.io.edf.**makeNaturalName** (*name*)

xrayutilities.io.fastscan module

modules to help with the analysis of FastScan data acquired at the ESRF. FastScan data are X-ray data (various detectors possible) acquired during scanning the sample in real space with a Piezo Scanner. The same functions might be used to analze traditional SPEC mesh scans.

The module provides three core classes:

* FastScan * FastScanCCD * FastScanSeries

where the first two are able to parse single mesh/FastScans when one is interested in data of a single channel detector or are detector and the last one is able to parse full series of such mesh scans with either type of detector

see examples/xrayutilities_kmap_ESRF.py for an example script

class xrayutilities.io.fastscan.**FastScan** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **object**
class to help parsing and treating fast scan data. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source.

grid2D (*nx*, *ny*, ***kwargs*)
function to grid the counter data and return the gridded X,Y and Intensity values.
Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))
gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

motorposition (*motorname*)
read the position of motor with name given by motorname from the data file. In case the motor is included in the data columns the returned object is an array with all the values from the file (although retrace clean is respected if already performed). In the case the motor is not moved during the scan only one value is returned.
Parameters

motorname: name of the motor for which the position is wanted

Returns

val: motor position(s) of motor with name motorname during the scan

parse ()
parse the specfile for the scan number specified in the constructor and store the needed informations in the object properties

retrace_clean ()
function to clean the data of the scan from retrace artifacts created by the zig-zag scanning motion of the piezo actuators the function cleans the xvalues, yvalues and data attribute of the FastScan object.

class xrayutilities.io.fastscan.**FastScanCCD** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **xrayutilities.io.fastscan.FastScan**
class to help parsing and treating fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed

getccdFileTemplate (*specscan*, *datadir=None*, *keepdir=0*, *numfmt='%04d'*)
function to extract the CCD file template string from the comment in the SPEC-file scan-header
Parameters

specscan: spec-scan object from which header the CCD directory should be extracted
datadir: the CCD filenames are usually parsed from the scan object. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.
keepdir: number of directories which should be taken from the specscan. (default: 0)
numfmt: format string for the CCD file number (optional)

Returns

fmtstr: format string for the CCD file name using one number to build the real file name

gridCCD (*nx, ny, ccdnr, roi=None, datadir=None, keepdir=0, nav=[1, 1], gridrange=None, filterfunc=None, imgoffset=0*)
function to grid the internal data and ccd files and return the gridded X,Y and DATA values. DATA represents a 4D with first two dimensions representing X,Y and the remaining two dimensions representing detector channels
Parameters

nx,ny: number of bins in x,y direction
ccdnr: array with ccd file numbers of length length(FastScanCCD.data) OR a string with the data column name for the file ccd-numbers

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

nav: number of detector pixel which will be averaged together (reduces the date size)

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

Returns

X,Y,DATA: regular x,y-grid as well as 4-dimensional data object

class xrayutilities.io.fastscan.**FastScanSeries** (*filenames*, *scannrs*, *nx*, *ny*, **args*, ***kwargs*)

Bases: **object**

class to help parsing and treating a series of fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed.

For the series of FastScans we assume that they are measured at different goniometer angles and therefore transform the data to reciprocal space.

align (*deltax*, *deltay*)

Since a sample drift or shift due to rotation often occurs between different FastScans it should be corrected before combining them. Since determining such a shift is not straight-forward in general the user needs to supply the routine with the shifts in order correct the x,y-values for the different FastScans. Such a routine could for example use the integrated CCD intensities and determine the shift using a cross-convolution.

Parameters

deltax: list of shifts in x-direction for every FastScan in the data structure

deltay: same for the y-direction

getCCDFrames (*posx*, *posy*, *typ='real'*)

function to determine the list of ccd-frame numbers for a specific real space position. The real space position must be within the data limits of the FastScanSeries otherwise an ValueError is thrown

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

Optional:

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

Returns

[[motorpos1, ccdnrs1], [motorpos2, ccdnrs2], ...] where motorposN is

from the N-ths FastScan in the series and ccdnrsN is the list of according CCD-frames

grid2Dall (*nx*, *ny*, ***kwargs*)

function to grid the counter data and return the gridded X,Y and Intensity values from all the FastScanSeries.

Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

gridRSM (*posx, posy, qnx, qny, qnz, qconv, roi=None, nav=[1, 1], typ='real', filterfunc=None, **kwargs*)

function to calculate the reciprocal space map at a certain x,y-position from a series of FastScan measurements it is necessary to specify the number of grid-oints for the reciprocal space map and the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qnx: number of points in the Qx direction of the gridded reciprocal space map

qny: same for y direction

qnz: same for z directino

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

Returns

Gridder3D object with gridded reciprocal space map

rawRSM (*posx, posy, qconv, roi=None, nav=[1, 1], typ='real', datadir=None, keepdir=0, filterfunc=None, **kwargs*)

function to return the reciprocal space map data at a certain x,y-position from a series of FastScan measurements. It necessary to give the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

Returns

Qx,qy,qz,ccddata,valuelist: raw data of the reciprocal space map and valuelist containing the ccdframe numbers and corresponding motor positions

read_motors ()
read motor values from the series of fast scans

retrace_clean ()
perform retrace clean for every FastScan in the series

xrayutilities.io.helper module

convenience functions to open files for various data file reader

these functions should be used in new parsers since they transparently allow to open gzipped and bzipped files

class xrayutilities.io.helper.**xu_h5open** (*f*, *mode='r'*)
Bases: **object**
helper object to decide if a HDF5 file has to be opened/closed when using with a 'with' statement.

xrayutilities.io.helper.**xu_open** (*filename*, *mode='rb'*)
function to open a file no matter if zipped or not. Files with extension '.gz' or '.bz2' are assumed to be compressed and transparently opened to read like usual files.
Parameters

filename: filename of the file to open (full including path)

mode: mode in which the file should be opened

Returns

file handle of the opened file
If the file does not exist an IOError is raised by the open routine, which is not caught within the function

xrayutilities.io.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 with

1. RoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point.
2. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

readImage (*filename*, *path=None*)
read image file and correct for dark- and flatfield in case the necessary data are available.
returned data = ((image data)-(darkfield))/flatfield*average(flatfield)
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed. supported extensions: .tif, .bin and .bin.xz

class xrayutilities.io.imagereader.**PerkinElmer** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse PerkinElmer CCD frames (*.tif) 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.**Pilatus100K** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse Dectris Pilatus 100k frames (*.tiff) to numpy arrays Ignore the header since it seems to contain no useful data

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.

class xrayutilities.io.imagereader.**TIFFRead** (*filename*, *path=None*)
Bases: **xrayutilities.io.imagereader.ImageReader**
class to Parse a TIFF file including extraction of information from the file header in order to determine the image size and data type
The data stored in the image are available in the 'data' property.

xrayutilities.io.imagereader.**get_tiff** (*filename*, *path=None*)
read tiff image file and return the data
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed.

xrayutilities.io.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*, *path=''*)
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*, *namespace=''*)

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.XRDMLFile class is used. The function can be used for parsing maps measured with the PIXCel 1D detector (and in limited way also for data acquired with a point detector -> see getxrdml_scan instead).
Parameters

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 usefull!

Returns

om,tt,psd: as flattened numpy arrays

Examples

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

xrayutilities.io.panalytical_xml.**getxrdml_scan** (*filetemplate*, **motors*, ***kwargs*)
parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLFile class is used. The function can be used for parsing arbitrary scans and will return the the motor values of the scan motor and additionally the positions of the motors given by in the "*motors" argument
Parameters

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

***motors: motor names to return: e.g.: 'Omega','2Theta',...**

one can also use abbreviations 'Omega' = 'om' = 'o' '2Theta' = 'tt' = 't' 'Chi' = 'c' 'Phi' = 'p'

****kwargs:**

scannrs: int or list of scan numbers
path: common path to the filenames

Returns

scanmot,mot1,mot2,...,detectorint: as flattened numpy arrays

Examples

```
>>> scanmot,om,tt,inte = xrayutilities.io.getxrdml_scan(
        "samplename_1.xrdml", 'om', 'tt', path="./data")
```

xrayutilities.io.pdcif module

class xrayutilities.io.pdcif.**pdCIF** (*filename*, *datacolumn=None*)
Bases: **object**
the class implements a primitive parser for pdCIF-like files. It reads every entry and collects the information in the header attribute. The first loop containing one of the intensity fields is assumed to be the data the user is interested in and is transfered to the data array which is stored as numpy record array the columns can be accessed by name

intensity fields:

_pd_meas_counts_total, _pd_meas_intensity_total, _pd_proc_intensity_total, _pd_proc_intensity_net, _pd_calc_intensity_total, _pd_calc_intensity_net

alternatively the data column name can be given as argument to the constructor

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

class xrayutilities.io.pdcif.**pdESG** (*filename*, *datacolumn=None*)
Bases: **xrayutilities.io.pdcif.pdCIF**
class for parsing multiple pdCIF loops in one file. This includes especially *.esg files which are supposed to consist of multiple loops of pdCIF data with equal length.
Upon parsing the class tries to combine the data of these different scans into a single data matrix -> same shape of subscan data is assumed

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

xrayutilities.io.pdcif.**remove_comments** (*line*, *sep='#'*)

xrayutilities.io.rigaku_ras module

class for reading data + header information from Rigaku RAS (3-column ASCII) files

Such datafiles are generated by the Smartlab Guidance software from Rigaku.

class xrayutilities.io.rigaku_ras.**RASFile** (*filename*, *path=None*)
Bases: **object**
Represents a RAS data file. The file is read during the constructor call
Required constructor arguments:

filename: a string with the name of the ras-file

keyword argument (optional):

path: path to the data file

Read ()
Read the data from the file

class xrayutilities.io.rigaku_ras.**RASScan** (*filename*, *pos*)
Bases: **object**
Represents a single Scan portion of a RAS data file. The scan is parsed during the constructor call
Required constructor arguments:

filename: file name of the data file
pos: seek position of the RAS_HEADER_START line

xrayutilities.io.rigaku_ras.**getras_scan** (*scanname*, *scannumbers*, **args*, ***kwargs*)
function to obtain the angular cooridinates as well as intensity values saved in RAS datafiles. Especially useful for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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: keyword arguments forwarded to RASFile function
Returns

rasdata

or

[ang1,ang2,...],rasdata:

angular positions are extracted from the respective scan header together with all the data values as stored in the data file (includes the intensities e.g. rasdata['int']).

Examples

```
>>> [om,tt],MAP = xu.io.getras_scan('text%05d.ras',36,'Omega','TwoTheta')
```

xrayutilities.io.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

xrayutilities.io.seifert module

a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two posibilities 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**

helper class to represent a Seifert (NJA) scan file header

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

Bases: **object**

Class to parse a Seifert (NJA) multiscan file

parse ()

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

Bases: **object**

Class to parse a single Seifert (NJA) scan file

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.

Parameters

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: can be either "map" (reciprocal space map measured with a regular Seifert job (default)) or "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

Examples

```
>>> 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 preceeding _.

xrayutilities.io.spec module

a 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**

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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

comp: activate 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**

class to parse a SPEC log file to find the command history

Parse ()

class xrayutilities.io.spec.**SPECScan** (*name*, *scannr*, *command*, *date*, *time*, *itime*, *colnames*, *hoffset*, *doffset*, *fname*, *imopnames*, *imopvalues*, *scan_status*)

Bases: **object**

Represents a single SPEC scan. This class is usually not called by the user directly but used via the SPECFile class.

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=''*, *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 ususally 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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

group: name or group object of the HDF5 group where to store the data

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

optattrs: a dictionary with optional attributes to store for the data

comp: activate 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 aguments:

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*, ***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:**

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 cooridinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially useful 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 h5py 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 ommited the first child node of h5f.root will be used

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

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']).

Examples

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

xrayutilities.io.spec.**getspec_scan** (*specf*, *scans*, **args*, ***kwargs*)

function to obtain the angular cooridinates as well as intensity values saved in a SPECFile. Especially useful to combine the data from multiple scans.
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

specf: SPECFile object

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

args: names of the motors and counters (strings)

keyword arguments:

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

Returns

[ang1,ang2,...]:

coordinates and counters from the SPEC file

Examples

```
>>> [om, tt, cnt2] = xu.io.getspec_scan(s, 36, 'omega', 'gamma',
                                        'Counter2')
```

xrayutilities.io.spec.**makeNaturalName** (*name*)

xrayutilities.io.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='/'*, *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

name: name of the group where to store the data

optional keyword arguments:

group: root group where to store the data

mcaname: Name of the MCA in the HDF5 file

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**

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

h5f: file object of a HDF5 file opened using h5py

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

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

omname: name of the omega motor (or its equivalent)

ttname: name of the two theta motor (or its equivalent)

****kwargs (optional):**

mca: name 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']).

Module contents

xrayutilities.materials package

Submodules

xrayutilities.materials.atom module

module containing the Atom class which handles the database access for atomic scattering factors and the atomic mass.

class xrayutilities.materials.atom.**Atom** (*name*, *num*)

Bases: **object**

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

function to calculate the atomic structure factor F

Parameters

q: momentum transfer

en: 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'*)

weight

xrayutilities.materials.cif module

class xrayutilities.materials.cif.**CIFFile** (*filename*, *digits=3*)

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.

xrayutilities.materials.database module

module to handle the access to the optical parameters database

class xrayutilities.materials.database.**DataBase** (*fname*)
Bases: **object**

Close ()
Close an opend 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*, *dset='default'*)
Obtain the f0 scattering factor component for a particular momentum transfer q.

required input argument:

q: single float value or numpy array
dset: specifies which dataset (different oxidation states) should be used

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*, *subset='default'*)

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
subset: specifies under which name the f0 values should be saved

SetF1F2 (*en*, *f1*, *f2*)
Set f1, f2 values for the active material.

required input arguments:

en: list or numpy array with energy in (eV)
f1: list or numpy array with f1 values
f2: list 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:

name: string with the name of the material

SetWeight (*weight*)
Save weight of the element as float

required input argument:

weight: atomic standard weight of the element (float)

xrayutilities.materials.database.**add_f0_from_intertab** (*db*, *itf*)
Read f0 data from International Tables of Crystallography and add it to the database.

xrayutilities.materials.database.**add_f0_from_xop** (*db*, *xop*)
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*, *hf*)
Read f1 and f2 data from Henke database and add it to the database.

xrayutilities.materials.database.**add_f1f2_from_kissel** (*db*, *kf*)
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. The mass of the natural isotope mixture is taken from the NIST data!

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

xrayutilities.materials.elements module

xrayutilities.materials.lattice module

module handling crystal lattice structures. A Lattice consists of unit cell parameters and a LatticeBase. It offers methods to calculate the reciprocal space position of Bragg peaks and their structure factor.

xrayutilities.materials.lattice.**AlGaAsLattice** (*aal*, *aga*, *aas*, *a*, *x*)

xrayutilities.materials.lattice.**BCCLattice** (*aa*, *a*)

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

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

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

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

xrayutilities.materials.lattice.**CubicLattice** (*a*, *base=None*)
Returns a Lattice object representing a cubic lattice.
Parameters

a: lattice parameter
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

xrayutilities.materials.lattice.**DiamondLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCSharedLattice** (*aa*, *ab*, *occa*, *occb*, *a*)

xrayutilities.materials.lattice.**GeTeRhombohedral** (*aa*, *ab*, *a*, *ang*, *x=0.237*)

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*)

xrayutilities.materials.lattice.**HexagonalLattice** (*a*, *c*, *base=None*)
Returns a Lattice object representing a hexagonal lattice.
Parameters

a: lattice parameter a
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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 and unit cell defined by three vectors.

ApplyStrain (*eps*)
Applies a certain strain on a lattice. The result is a change in the base vectors. The full strain matrix (3x3) needs to be given. .. note:: Note: NO elastic response of the material will be considered!

requiered input arguments:

eps: a 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 (angstrom^3)

a

a1

a2

a3

alpha

b

beta

c

gamma

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
Parameters

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*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.**MagnetiteLattice** (*aa*, *ab*, *ac*, *a*, *x=0.255*)

xrayutilities.materials.lattice.**MonoclinicLattice** (*a*, *b*, *c*, *beta*, *base=None*)
Returns a Lattice object representing a hexagonal lattice.
Parameters

a:	lattice parameter a
b:	lattice parameter b
c:	lattice parameter c
beta:	monoclinic unit cell angle beta (deg)
base:	instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

xrayutilities.materials.lattice.**NiAsLattice** (*aa*, *ab*, *a*, *c*, *biso=0.0*)

xrayutilities.materials.lattice.**OrthorhombicLattice** (*a*, *b*, *c*, *base=None*)
Returns a Lattice object representing a tetragonal lattice.
Parameters

a: lattice parameter a
b: lattice parameter b
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

`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*)
creates the primitive unit cell of a RockSalt structure. For the more commonly used cubic reprentation see RockSalt_Cubic_Lattice

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

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

`xrayutilities.materials.lattice.`**`SiGeLattice`** (*asi*, *age*, *a*, *xge*)

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

`xrayutilities.materials.lattice.`**`TetragonalLattice`** (*a*, *c*, *base=None*)
Returns a Lattice object representing a tetragonal lattice.
Parameters

a: lattice parameter a
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

`xrayutilities.materials.lattice.`**`TriclinicLattice`** (*a*, *b*, *c*, *alpha*, *beta*, *gamma*, *base=None*)

`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*)

xrayutilities.materials.material module

Classes decribing materials. Materials are devided with respect to their crystalline state in either Amorphous or Crystal types. While for most materials their crystalline state is defined few materials are also included as amorphous which can be useful for calculation of their optical properties.

class `xrayutilities.materials.material.`**`Alloy`** (*matA*, *matB*, *x*)
Bases: **`xrayutilities.materials.material.Crystal`**

`RelaxationTriangle` **(*hkl*, *sub*, *exp*)**
function which returns the relaxation trianlge for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class
Parameters

hkl: Miller Indices
sub: substrate material or lattice constant (Instance of Crystal 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

class xrayutilities.materials.material.**Amorphous** (*name*, *density*, *atoms=None*, *cij=None*)
Bases: **xrayutilities.materials.material.Material**
amorphous materials are described by this class

beta (*en='config'*)
function to calculate the imaginary part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

delta (*en='config'*)
function to calculate the real part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

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.**Crystal** (*name*, *lat*, *cij=None*, *thetaDebye=None*)
Bases: **xrayutilities.materials.material.Material**
Crystalline materials are described by this class

ApplyStrain (*strain*)
Applies a certain strain on the lattice of the material. The result is a change in the base vectors of the real space as well as reciprocal space lattice. The full strain matrix (3x3) needs to be given. Note: NO elastic response of the material will be considered!

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.
Parameters

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
Parameters

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
Parameters

q0: vectorial momentum transfer (vectors as list,tuple or numpy array are valid)
en: list, tuple or array of energy values in eV
temp: temperature 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
Parameters

q: vectorial 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)])
en0: energy value in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature 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)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 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
Parameters

q: momentum transfer in (1/A)
en: xray energy in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature used for Debye-Waller-factor calculation
polarization: either 'S' (default) sigma or 'P' pi polarization

Returns

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

dTheta (*Q*, *en='config'*)
function to calculate the refractive peak shift
Parameters

Q: momentum transfer (1/A)
en: x-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaTheta: peak 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)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

density
calculates the mass density of an material from the mass of the atoms in the unit cell.
Returns
mass density in kg/m^3

distances ()
function to obtain distances of atoms in the crystal up to the unit cell size (largest value of a,b,c is the cut-off)
returns a list of tuples with distance d and number of occurence n [(d1,n1),(d2,n2),...]

Note

Note: if the base of the material is empty the list will be empty

environment (pos*, ***kwargs*)**
Returns a list of neighboring atoms for a given position within the the unit cell.
Parameters

pos: list or numpy array with the fractional coordinated in the unit cell

keyword arguments:

maxdist: maximum distance wanted in the list of neighbors :(default: 7)

Returns

list of tuples with (distance,atomType,multiplicity) giving distance (sorted) and type of neighboring atoms together with the amount of atoms at the given distance

classmethod **fromCIF** (*ciffilename*)

Create a Crystal from a CIF file. Name and

Parameters

ciffilename: filename of the CIF file

Returns

Crystal instance

planeDistance (*hkl)

determines the lattice plane spacing for the planes specified by (hkl)

Parameters

h,k,l: Miller indices of the lattice planes given either as list,tuple or seperate arguments

Returns

d: the lattice plane spacing as float

Examples

```
>>> xu.materials.Si.planeDistance(0,0,4)
1.3577600000000001
```

or

```
>>> xu.materials.Si.planeDistance((1,1,1))
3.1356124059796255
```

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

Parameters

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 symetric peak. As an additional input the substrates lattice parameter and the degree of relaxation must be given

Parameters

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

Parameters

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'`*, *`base=None`*)

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

Parameters

a,b,c: unit cell extenstions (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

base: instance of LatticeBase

returns a Crystal 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

Parameters

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`*, *`cij=None`*)

Bases: **`object`**

base class for all Materials. common properties of amorphous and crystalline materials are described by this class from which Amorphous and Crystal are derived from.

`beta (en='config')`

`chi0 (en='config')`

calculates the complex chi_0 values often needed in simulations. They are closely related to delta and beta (n = 1 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

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

calculate critical angle for total external reflection

Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

deg: return angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

delta (*en='config'*)

density

idx_refraction (*en='config'*)
function to calculate the complex index of refraction of a material in the x-ray range
Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

xrayutilities.materials.material.**PseudomorphicMaterial** (*sub*, *layer*, *relaxation=0*, *trans=None*)
This function returns a material whos lattice is pseudomorphic on a particular substrate material. The two materials must have similar unit cell definitions for the algorithm to work correctly, i.e. it does not work for combiniations of materials with different lattice symmetry.
Parameters

sub: substrate material

layer: bulk material of the layer

relaxation: degree of relaxation 0: pseudomorphic, 1: relaxed :(default: 0)

trans: Transformation which transforms lattice directions into a surface orientated coordinate frame (x,y inplane, z out of plane). If None a (001) surface geometry of a cubic material is assumed.

Returns
An instance of Crystal holding the new pseudomorphically strained material.

xrayutilities.materials.material.**WZTensorFromCub** (*c11ZB*, *c12ZB*, *c44ZB*)
Determines the hexagonal elastic tensor from the values of the cubic elastic tensor under the assumptions presented in Phys. Rev. B 6, 4546 (1972), which are valid for the WZ <-> ZB polymorphs.
Parameters

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

Returns

6x6 matrix with elastic constants

Implementation according to a patch submitted by Julian Stangl

xrayutilities.materials.material.**index_map_ij2ijkl** (*ij*)

xrayutilities.materials.material.**index_map_ijkl2ij** (*i*, *j*)

xrayutilities.materials.predefined_materials module

class xrayutilities.materials.predefined_materials.**AlGaAs** (*x*)
Bases: **xrayutilities.materials.material.CubicAlloy**

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

Module contents

xrayutilities.math package

Submodules

xrayutilities.math.algebra module

module providing analytic algebraic functions not implemented in scipy or any other dependency of xrayutilities. In particular the analytic solution of a quartic equation which is needed for the solution of the dynamic scattering equations.

`xrayutilities.math.algebra.`**`solve_quartic`** (*a4*, *a3*, *a2*, *a1*, *a0*)

analytic solution [1] of the general quartic equation. The solved equation takes the form:
a4*z**4 + a3*z**3 + a2*z**2 + a1*z + a0

Returns

tuple of the four (complex) solutions of aboves equation.

[1] http://mathworld.wolfram.com/QuarticEquation.html

xrayutilities.math.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,y:	data coordinates (do NOT need to be regularly spaced)
data:	data set used for fitting (e.g. intensity at the data coords)
start:	set of starting parameters for the fit used as first parameter of function fit_function
drange:	limits 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_function:	function 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=300*)

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

Parameters

xdata:	xcoordinates of the data to be fitted
ydata:	ycoordinates of the data which should be fit

keyword parameters:

iparams:	initial paramters for the fit, determined automatically if not given
maxit:	maximal 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

`xrayutilities.math.fit.`**`linregress`** (*x*, *y*)

fast linregress to avoid usage of scipy.stats which is slow!

Parameters

x,y: data coordinates and values

Returns

p, rsq: parameters of the linear fit (slope, offest) and the R^2 value

Examples

```
>>> (k, d), R2 = xu.math.linregress(x, y)
```

xrayutilities.math.fit.**multGaussFit** (**args*, ***kwargs*)

convenience function to keep API stable see multPeakFit for documentation

xrayutilities.math.fit.**multGaussPlot** (**args*, ***kwargs*)

convenience function to keep API stable see multPeakPlot for documentation

xrayutilities.math.fit.**multPeakFit** (*x*, *data*, *peakpos*, *peakwidth*, *dranges=None*, *peaktype='Gaussian'*)

function to fit multiple Gaussian/Lorentzian peaks with linear background to a set of data

Parameters

x: x-coordinate of the data

data: data array with same length as x

peakpos: initial parameters for the peak positions

peakwidth: initial values for the peak width

dranges: list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as peakpos

peaktype: type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'

Returns

pos,sigma,amp,background

Pos: list of peak positions derived by the fit

Sigma: list of peak width derived by the fit

Amp: list of amplitudes of the peaks derived by the fit

Background: array of background values at positions x

xrayutilities.math.fit.**multPeakPlot** (*x*, *fpos*, *fwidth*, *famp*, *background*, *dranges=None*, *peaktype='Gaussian'*, *fig='xu_plot'*, *fact=1.0*)

function to plot multiple Gaussian/Lorentz peaks with background values given by an array

Parameters

x: x-coordinate of the data

fpos: list of positions of the peaks

fwidth: list of width of the peaks

famp: list of amplitudes of the peaks

background: array with background values

dranges: list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as fpos

peaktype: type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'

fig: matplotlib figure number or name

fact: factor to use as multiplicator in the plot

xrayutilities.math.fit.**peak_fit** (*xdata*, *ydata*, *iparams=[*, *]*, *peaktype='Gauss'*, *maxit=300*, *background='constant'*, *plot=False*, *func_out=False*, *debug=False*)

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

Parameters

xdata: xcoordinates of the data to be fitted

ydata: ycoordinates of the data which should be fit

keyword parameters:

iparams: initial paramters for the fit, determined automatically if not specified

peaktype: type of peak to fit: 'Gauss', 'Lorentz', 'PseudoVoigt', 'PseudoVoigtAsym'

maxit: maximal iteration number of the fit

background: type of background, either 'constant' or 'linear'

plot: flag to ask for a plot to visually judge the fit. If plot is a string it will be used as figure name, which makes reusing the figures easier.

func_out: returns the fitted function, which takes the independent variables as only argument (f(x))

Returns

params,sd_params,itlim[,fitfunc]

the parameters as defined in function Gauss1d/Lorentz1d/PseudoVoigt1d/ PseudoVoigt1dasym(x, *param). In the case of linear background one more parameter is included! For every parameter the corresponding errors of the fit 'sd_params' are returned. A boolean flag 'itlim', which is False in the case of a successful fit is added by default. Further the function used in the fit can be returned (see func_out).

xrayutilities.math.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
Examples
Calling with a list of parameters needs a call looking as shown below (note the '*') or explicit listing of the parameters: >>> Gauss1d(x,*p) >>> Gauss1d(numpy.linspace(0,10,100), 5, 1, 1e3, 0)

`xrayutilities.math.functions.`**`Gauss1dArea`** (**p*)

function to calculate the area of a Gauss function with neglected background
Parameters

p: list of parameters of the Gauss-function [XCEN,SIGMA,AMP,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

`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.**Gauss2dArea** (**p*)
function to calculate the area of a 2D Gauss function with neglected background
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,ANGLE,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

xrayutilities.math.functions.**Gauss3d** (*x*, *y*, *z*, **p*)
function to calculate a general three dimensional Gaussian
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,ZCEN,SIGMAX,SIGMAY,SIGMAZ,AMP,BACKGROUND] SIGMA = FWHM / (2*sqrt(2*log(2)))

x,y,z: coordinate(s) where the function should be evaluated

Returns
the value of the Gaussian described by the parameters p at positions (x,y,z)

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: 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.**Lorentz1dArea** (**p*)
function to calculate the area of a Lorentz function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

Returns
the area of the Lorentzian described by the parameters p

xrayutilities.math.functions.**Lorentz1d_der_p** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect the parameters p
for parameter description see Lorentz1d

xrayutilities.math.functions.**Lorentz1d_der_x** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect to x
for parameter description see Lorentz1d

xrayutilities.math.functions.**Lorentz2d** (*x*, *y*, **p*)
function to calculate a general two dimensional Lorentzian
Parameters

p: list 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,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.**NormGauss1d** (*x*, **p*)
function to calculate a normalized one dimensional Gaussian
Parameters

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

x: coordinate(s) where the function should be evaluated

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

xrayutilities.math.functions.**PseudoVoigt1d** (*x*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

xrayutilities.math.functions.**PseudoVoigt1dArea** (**p*)
function to calculate the area of a pseudo Voigt function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the area of the PseudoVoigt described by the parameters p

xrayutilities.math.functions.**PseudoVoigt1d_der_p** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect the parameters p
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1d_der_x** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect to x
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1dasym** (*x*, **p*)
function to calculate an asymmetric pseudo Voigt function as linear combination of asymmetric Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHMLEFT,FWHMRIGHT,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

xrayutilities.math.functions.**PseudoVoigt2d** (*x*, *y*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak in two dimensions
Parameters

x,y: coordinate(s) where the function should be evaluated

p: list of parameters of the pseudo Voigt-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the value of the PseudoVoigt 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

p: list of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2, SIGMAX2,SIGMAY2,AMP2,ANGLE2,BACKGROUND] 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.`**`heaviside`** (*x*)
Heaviside step function for numpy arrays
Parameters

x: any scalar of ndarray object

Returns

s: Heaviside step function evaluated for all values of x

`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

data: 1d numpy array with experimental data

threshold: threshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.`**`multPeak1d`** (*x*, *`*args`*)
function to calculate the sum of multiple peaks in 1D. the peaks can be of different type and a background function (polynom) can also be included.
Parameters

x: coordinate where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'a': asym. PseudoVoigt, 'p': polynom the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss1d, math.Lorentz1d, math.PseudoVoigt1d, math.PseudoVoigt1dasym, and numpy.polyval for details of the different function types.

Returns

value of the sum of functions at position x

`xrayutilities.math.functions.`**`multPeak2d`** (*x*, *y*, *`*args`*)

function to calculate the sum of multiple peaks in 2D. the peaks can be of different type and a background function (polynom) can also be included.
Parameters

x,y: coordinates where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'c': constant the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss2d, math.Lorentz2d, math.PseudoVoigt2d for details of the different function types. The constant accepts a single float which will be added to the data

Returns

value of the sum of functions at position (x,y)

`xrayutilities.math.functions.`**`smooth`** (*x*, *n*)
function to smooth an array of data by averaging N adjacent data points
Parameters

x: 1D data array

n: number of data points to average

Returns

xsmooth: smoothed array with same length as x

xrayutilities.math.misc module

`xrayutilities.math.misc.`**`center_of_mass`** (*pos*, *data*, *background='none'*, *full_output=False*)
function to determine the center of mass of an array
Parameters

pos: position of the data points

data: data values

background: type of background, either 'none', 'constant' or 'linear'

full_output: return background cleaned data and background-parameters

Returns

center of mass position (single float)

`xrayutilities.math.misc.`**`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)
Parameters

pos: position of the data points

data: data values

Returns

fwhm value (single float)

xrayutilities.math.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.

class `xrayutilities.math.transforms.`**`AxisToZ_keepXY`** (*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/y-axis of the new coordinate frame is created to be similar to the old x and y directions. This variant of AxisToZ assumes that the new Z-axis has its main component along the Z-direction

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*, *rank=1*)
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 size of the transformation matrix.

rank: rank of the supplied object. allowed values are 1, 2, and 4

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 radiants.

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 radiants.

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 radiants.

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
Parameters

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

Examples

```
>>> 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

xrayutilities.math.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)*norm(v2)*cos(alpha*)

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 radiants

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

Module contents

xrayutilities.simpack package

Submodules

xrayutilities.simpack.fit module

`xrayutilities.simpack.fit.`**`fit_xrr`** (*`reflmod`*, *`params`*, *`ai`*, *`data=None`*, *`eps=None`*, *`xmin=-inf`*, *`xmax=inf`*, *`plot=False`*, *`verbose=False`*, *`elog=True`*, *`maxfev=500`*)
optimize function for a Reflectivity Model using lmfit. The fitting parameters must be specified as instance of lmfits Parameters class.
Parameters

reflmod: preconfigured SpecularReflectivityModel

params: instance of lmfits Parameters class. For every layer the parameters '{}_thickness', '{}_roughness', '{}_density', with '{}' representing the layer name are supported. In addition the setup parameters: - 'I0' primary beam intensity - 'background' background added to the simulation - 'sample_width' size of the sample along the beam - 'beam_width' width of the beam in the same units - 'resolution_width' width of the resolution function in deg - 'shift' experimental shift of the incidence angle array

ai: array of incidence angles for the calculation

data: experimental data which should be fitted

eps: (optional) error bar of the data

xmin: minimum value of ai which should be used. a mask is generated to cut away other data

xmax: maximum value of ai which should be used. a mask is generated to cut away other data

plot: flag to decide wheter an plot should be created showing the fit's progress. If plot is a string it will be used as figure name, which makes reusing the figures easier.

verbose: flag to tell if the variation of the fitting error should be output during the fit.

elog: logarithmic error during the fit

maxfev: maximum number of function evaluations during the leastsq optimization

Returns

res: MinimizerResult object from lmfit, which contains the fitted parameters in res.params (see res.params.pretty_print) or try lmfit.report_fit(res)

xrayutilities.simpack.models module

class xrayutilities.simpack.models.**DynamicalModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.SimpleDynamicalCoplanarModel**

Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a generalized 2-beam theory (4 tiepoints, S and P polarizations)

The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*)

performs the actual diffraction calculation for the specified incidence angles and uses an analytic solution for the quartic dispersion equation

Parameters

alphai: vector of incidence angles (deg)

hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)

geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**KinematicalModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.LayerModel**

Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of one (hkl) Bragg peak, however considers the variation of the structure factor for different 'q'. The surface geometry is specified using the Experiment-object given to the constructor.

init_chi0 ()

calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness does NOT require this!)

simulate (*qz*, *hkl*, *absorption=False*, *refraction=False*)

performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a single Bragg peak.

Parameters

qz: simulation positions along qz

hkl: Miller indices of the Bragg peak whos truncation rod should be calculated

absorption: flag to tell if absorption correction should be used

refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**KinematicalMultiBeamModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.KinematicalModel**

Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of several Bragg peaks on the truncation rod and considers the variation of the structure factor. In order to use a analytical description for the kinematic diffraction signal all layer thicknesses are changed to a multiple of the respective lattice parameter along qz. Therefore this description only works for (001) surfaces.

simulate (*qz*, *hkl*, *absorption=False*, *refraction=True*)

performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a full truncation rod

Parameters

qz: simulation positions along qz

hkl: Miller indices of the Bragg peak whos truncation rod should be calculated

absorption: flag to tell if absorption correction should be used

refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**LayerModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.Model**

generic model class from which further thin film models can be derived from

class xrayutilities.simpack.models.**Model** (*experiment*, ***kwargs*)

Bases: **object**

generic model class from which further models can be derived from

convolute_resolution (*x*, *y*)

convolve simulation result with a Gaussian resolution function

Parameters

x: x-values of the simulation, units of x also decide about the unit of the resolution_width parameter

y: y-values of the simulation

Returns

convoluted y-data with same shape as y

scale_simulation (*y*)

scale simulation result with primary beam flux/intensity and add a background.

Parameters

y: y-values of the simulation

Returns

scaled y values

class xrayutilities.simpack.models.**SimpleDynamicalCoplanarModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.KinematicalModel**

Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a simplified 2-beam theory (2 tiepoints, S and P polarizations)

No restrictions are made for the surface orientation.

The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

Note

Note: This model should not be used in real life scenarios since the made approximations severely fail for distances far from the reference position.

get_polarizations ()

return list of polarizations which should be calculated

join_polarizations (*Is*, *Ip*)

method to calculate the total diffracted intensity from the intensities of S and P-polarization.

set_hkl (hkl*)**

To speed up future calculations of the same Bragg peak optical parameters can be pre-calculated using this function.

Parameters

hkl: Miller indices of the Bragg peak for the calculation

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*, *idxref=1*)
performs the actual diffraction calculation for the specified incidence angles.
Parameters

alphai: vector of incidence angles (deg)
hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)
geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence
idxref: index of the reference layer. In order to get accurate peak position of the film peak you want this to be the index of the film peak (default: 1). For the substrate use 0.

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**SpecularReflectivityModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.LayerModel**
model for specular reflectivity calculations

densityprofile (*nz*, *plot=False*)
calculates the electron density of the layerstack from the thickness and roughness of the individual layers
Parameters

nz: number of values on which the profile should be calculated
plot: flag to tell if a plot of the profile should be created

Returns

z, eprof: coordinates and electron profile. z = 0 corresponds to the
surface

init_cd ()
calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness and roughness do NOT require this!)

simulate (*alphai*)
performs the actual reflectivity calculation for the specified incidence angles
Parameters

alphai: vector of incidence angles

Returns
vector of intensities of the reflectivity signal

xrayutilities.simpack.models.**startdelta** (*start*, *delta*, *num*)

xrayutilities.simpack.smaterials module

class xrayutilities.simpack.smaterials.**CrystalStack** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.LayerStack**
extends the built in list type to enable building a stack of crystalline Layers by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**GradedLayerStack** (*alloy*, *xfrom*, *xto*, *nsteps*, *thickness*, ***kwargs*)
Bases: **xrayutilities.simpack.smaterials.CrystalStack**
generates a sequence of layers with a gradient in chemical composition

class xrayutilities.simpack.smaterials.**Layer** (*material*, *thickness*, ***kwargs*)
Bases: **xrayutilities.simpack.smaterials.SMaterial**
Object describing part of a thin film sample. The properties of a layer :are:

Material:	an xrayutilties material describing optical and crystal properties of the thin film
Thickness:	film thickness in Angstrom
Roughness:	root mean square roughness of the top interface in Angstrom

class xrayutilities.simpack.smaterials.**LayerStack** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.MaterialList**
extends the built in list type to enable building a stack of Layer by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**MaterialList** (*name*, **args*)
Bases: **_abcoll.MutableSequence**
class representing the basics of a list of materials for simulations within xrayutilities. It extends the built in list type.

check (*v*)

insert (*i*, *v*)

class xrayutilities.simpack.smaterials.**PseudomorphicStack001** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.CrystalStack**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 001 and materials must be cubic/tetragonal.

insert (*i*, *v*)

make_epitaxial (*i*)

trans = *<xrayutilities.math.transforms.Transform object at 0x7f2db1e4ae50>*

class xrayutilities.simpack.smaterials.**PseudomorphicStack111** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.PseudomorphicStack001**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 111 and materials must be cubic.

trans = *<xrayutilities.math.transforms.CoordinateTransform object at 0x7f2db0fe3090>*

class xrayutilities.simpack.smaterials.**SMaterial** (*material*, ***kwargs*)
Bases: **object**
Simulation Material. Extends the xrayutilities Materials by properties needed for simulations

Module contents

simulation subpackage of xrayutilities.

This package provides possibilities to simulate X-ray diffraction and reflectivity curves of thin film samples. It could be extended for more general use in future if there is demand for that.

In addition it provides a fitting routine for reflectivity data which is based on lmfit.

Submodules

xrayutilities.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.

xrayutilities.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)

Attibutes

expr -- input expression in which the error occurred :msg: -- explanation of the error

xrayutilities.experiment module

module helping with planning and analyzing experiments. various classes are provided for describing experimental geometries, calculationof angular coordinates of Bragg reflections, conversion of angular coordinates to Q-space and determination of powder diffraction peak positions.

The strength of the module is the versatile QConversion module which can be configured to describe almost any goniometer geometry.

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 Crystal. You can specify the matrix B (default identiy matrix) shape needs to be (3,3)
mat:	Crystal 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
U:	orientation matrix U can be given. If none is given the orientation defined in the Experiment class is used.
dettype:	detector type: one of ('point', 'linear', 'area') decides which routine of Ang2Q to call. default 'point'
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
wl:	x-ray wavelength in angstroem (default: self._wl)
en:	x-ray energy in eV (default: converted self._wl)
deg:	flag to tell if angles are passed as degree (default: True)
sampledis:	sample displacement vector in relative units of the detector distance (default: (0, 0, 0))

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

q: list or numpy array with the reciprocal space position

optional keyword arguments:

deg: True/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. This is for example necessary before any Q2Ang-conversion can be performed.

Parameters

v: 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

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

Using this class the default sample surface orientation is determined by the inner most sample rotation (which is usually the azimuth motor).

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. However, if one angle is always the same its enough to give one scalar value.

****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)

deg: flag 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/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 [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.**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,beta: sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length. Howevver, if one angle is always the same its enough to give one scalar value.

****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 3. Used angles are than ai,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)

deg: flag 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. However, if one angle is always the same its enough to give one scalar value.

****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)

deg: flag 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. The coplanar scattering angles correspond to a goniometer with sample rotations ['x+','y+','z-'] and detector rotation 'x+' and primary beam along y. This is a standard four circle diffractometer.
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/Flase (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 geometries return [omega,0,phi,twotheta]
- "realTilt" general geometry with angles determined by q-coordinates (tilt); returns [omega,chi,phi,twotheta]

default: self.geometry

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

mat: Crystal object; needed to obtain its optical properties for refraction correction, otherwise not used

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

fi,fd: if 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]

omega: incidence angle with respect to surface

chi: sample tilt for the case of non-coplanar geometry

phi: sample azimuth with respect to inplane reference direction

twotheta: scattering 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_i: offset of the incidence beam from the scattering plane due to refraction

pdi_d: offset ot 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,tt: sample and detector angles as numpy array, lists or Scalars must be given. All arguments must have the same shape or length. However, if one angle is always the same its enough to give one scalar value.

****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 om,chi,phi,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)
deg: flag 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/Flase (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*)
Convolutes 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 and X-ray energy. Both angular scans (where some goniometer angles change during data acquisition) and energy scans (where the energy is varied during acquisition) as well as mixed cases can be treated.
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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)
roi: region of interest for the detector pixels; e.g. [100, 900, 200, 800] (default: self._area_roi)
Nav: number of channels to average to reduce data size e.g. [2, 2] (default: self._area_nav)
wl: x-ray wavelength in angstroem (default: self._wl)
en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!
deg: flag to tell if angles are passed as degree (default: True)
sampledis: sample displacement vector in same units as the detector distance (default: (0, 0, 0))

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 varing

detectorAxis
property handler for _detectorAxis
Returns

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

energy

getDetectorDistance (args*, ***kwargs*)**

obtains the detector distance by applying the detector arm movements. This is especially interesting for the case of 1 or 2D detectors to perform certain geometric corrections.

Parameters

***args: detector angles. Only detector arm angles as described by the**

detectorAxis attribute must be given.

****kwargs: optional keyword arguments**

dim: dimension of the detector for which the position should be determined

roi: region of interest for the detector pixels; :(default: self._area_roi/self._linear_roi)

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

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

Returns

numpy array with the detector distance

getDetectorPos (args*, ***kwargs*)**

obtains the detector position vector by applying the detector arm rotations.

Parameters

***args: detector angles. Only detector arm angles as described by the**

detectorAxis attribute must be given.

****kwargs: optional keyword arguments**

dim: dimension of the detector for which the position should be determined

roi: region of interest for the detector pixels; :(default: self._area_roi/self._linear_roi)

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

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

Returns

numpy array of length 3 with vector components of the detector direction. The length of the vector is k.

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

detectorDir1: direction of the detector (along the pixel direction 1); e.g. 'z+' means higher pixel numbers at larger z positions

detectorDir2: direction of the detector (along the pixel direction 2); e.g. 'x+'

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

Nch1: number of detector pixels along direction 1

Nch2: number 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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)

en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!

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

sampledis: sample displacement vector in same units as the detector distance (default: (0, 0, 0))

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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)

en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!

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

sampledis: sample displacement vector in relative units of the detector distance (default: (0,0,0))

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][+-]/

transformSample2Lab (*vector*, **args*)
transforms a vector from the sample coordinate frame to the laboratory coordinate system by applying the sample rotations from inner to outer circle.
Parameters

vector: vector to transform (sequence, list, numpy array)
args: goniometer angles (sample angles or full goniometer angles can be given. If more angles than the sample circles are given they will be ignored)

Returns

rotated vector as numpy.array

wavelength

xrayutilities.gridder module

class xrayutilities.gridder.**FuzzyGridder1D** (*nx*)
Bases: **xrayutilities.gridder.Gridder1D**
An 1D binning class considering every data point to have a finite width. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite width (e.g. X-ray data from a 1D detector).

class xrayutilities.gridder.**Gridder**
Bases: **object**
Basis class for gridders in xrayutilities. A gridder is a function mapping irregular spaced data onto a regular grid by binning the data into equally sized elements.
There are different ways of defining the regular grid of a Gridder. In xrayutilities the data bins extend beyond the data range in the input data, but the given position being the center of these bins, extends from the minimum to the maximum of the data! The main motivation for this was to create a Gridder, which when feeded with N equidistant data points and gridded with N bins would not change the data position (not the case with numpy.histogramm functions!). Of course this leads to the fact that for homogeneous point density the first and last bin in any direction are not filled as the other bins.
A different definition is used by numpy histogram functions where the bins extend only to the end of the data range. (see numpy histogram, histrogram2d, ...)

Clear ()
Clear so far gridded data to reuse this instance of the Gridder

KeepData (*bool*)

Normalize (*bool*)
set or unset the normalization flag. Normalization needs to be done to obtain proper gridding but may want to be disabled in certain cases when sequential gridding is performed

data
return gridded data (performs normalization if switched on)

class xrayutilities.gridder.**Gridder1D** (*nx*)
Bases: **xrayutilities.gridder.Gridder**

dataRange (*min*, *max*, *fixed=True*)
define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored
Parameters

min: minimum value of the gridding range
max: maximum value of the gridding range

fixed: flag to turn fixed range gridding on (True (default)) or off (False)

xaxis
Returns the xaxis of the gridder the returned values correspond to the center of the data bins used by the gridding algorithm

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.**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

class xrayutilities.gridder.**npyGridder1D** (*nx*)
Bases: **xrayutilities.gridder.Gridder1D**

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

xrayutilities.gridder2d module

class xrayutilities.gridder2d.**FuzzyGridder2D** (*nx*, *ny*)
Bases: **xrayutilities.gridder2d.Gridder2D**
An 2D binning class considering every data point to have a finite area. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite size (e.g. X-ray data from a 2D detector or reciprocal space maps measured with point/linear detector).
Currently only a rectangular area can be considered during the gridding.

class xrayutilities.gridder2d.**Gridder2D** (*nx*, *ny*)
Bases: **xrayutilities.gridder.Gridder**

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

dataRange (*xmin*, *xmax*, *ymin*, *ymax*, *fixed=True*)
define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored
Parameters

xmin,ymin: minimum value of the gridding range in x,y
xmax,ymax: maximum value of the gridding range in x,y

fixed: flag to turn fixed range gridding on (True (default)) or off (False)

xaxis

xmatrix

yaxis

ymatrix

class xrayutilities.gridder2d.**Gridder2DList** (*nx*, *ny*)
Bases: **xrayutilities.gridder2d.Gridder2D**
special version of a 2D gridder which performs no actual averaging of the data in one grid/bin but just collects the data-objects belonging to one bin for further treatment by the user

Clear ()

data
return gridded data, in this special version no normalization is defined!

xrayutilities.gridder3d module

class xrayutilities.gridder3d.**FuzzyGridder3D** (*nx*, *ny*, *nz*)
Bases: **xrayutilities.gridder3d.Gridder3D**
An 3D binning class considering every data point to have a finite volume. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite size.
Currently only a quader can be considered as volume during the gridding.

class xrayutilities.gridder3d.**Gridder3D** (*nx*, *ny*, *nz*)
Bases: **xrayutilities.gridder.Gridder**

SetResolution (*nx*, *ny*, *nz*)

dataRange (*xmin*, *xmax*, *ymin*, *ymax*, *zmin*, *zmax*, *fixed=True*)
define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored
Parameters

xmin,ymin,zmin: minimum value of the gridding range in x,y,z

xmax,ymax,zmax: maximum value of the gridding range in x,y,z

fixed: flag to turn fixed range gridding on (True (default)) or off (False)

xaxis

xmatrix

yaxis

ymatrix

zaxis

zmatrix

xrayutilities.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

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
Parameters

data: data which should be contracted (length N)
Nav: number 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
Parameters

data2d: array of 2D data shape (N,M)
Nav1,2: a field of (Nav1 x Nav2) values is contracted

****kwargs: optional keyword argument**

roi: region 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 serveral PSD spectra all data are used therefore the last cell used for averaging may differ in size
Parameters

psddata: array of 2D data shape (Nspectra,Nchannels)

Nav: number of channels which should be averaged

****kwargs: optional keyword argument**

roi: region 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))

xrayutilities.q2ang_fit module

Module provides functions to convert a q-vector from reciprocal space to angular space. a simple implementation uses scipy optimize routines to perform a fit for a arbitrary goniometer.

The user is, however, expected to use the bounds variable to put restrictions to the number of free angles to obtain reproducible results. In general only 3 angles are needed to fit an arbitrary q-vector (2 sample + 1 detector angles or 1 sample + 2 detector). More complicated restrictions can be implemented using the lmfit package. (done upon request!)

The function is based on a fitting routine. For a specific goniometer also analytic expressions from literature can be used as they are implemented in the predefined experimental classes HXRD, NonCOP, and GID.

`Q2AngFit(qvec, expclass, bounds=None, ormat=array([[ 1., 0., 0.],`
`[ 0., 1., 0.],`
`[ 0., 0., 1.]]), startvalues=None, constraints=())`
Functions to convert a q-vector from reciprocal space to angular space. This implementation uses scipy optimize routines to perform a fit for a goniometer with arbitrary number of goniometer angles.
The user *must* use the bounds variable to put restrictions to the number of free angles to obtain reproducible results. In general only 3 angles are needed to fit an arbitrary q-vector (2 sample + 1 detector angles or 1 sample + 2 detector).
Parameters

qvec: q-vector for which the angular positions should be calculated

expclass: experimental class used to define the goniometer for which the angles should be calculated.

keyword arguments(optional):

bounds: list of bounds of the goniometer angles. The number of bounds must correspond to the number of goniometer angles in the expclass. Angles can also be fixed by supplying only one value for a particular angle. e.g.: ((low, up), fix, (low2, up2), (low3, up3))

ormat: orientation matrix of the sample to be used in the conversion

startvalues: start values for the fit, which can significantly speed up the conversion. The number of values must correspond to the number of angles in the goniometer of the expclass

constraints: sequence of constraint dictionaries. This allows applying arbitrary (e.g. pseudo-angle) contraints by supplying according constraint functions. (see scipy.optimize.minimize). The supplied function will be called with the arguments (angles, qvec, Experiment, U).

Returns

fittedangles, qerror, errcode:

list of fitted goniometer angles, the error in reciprocal space and the errcode of the scipy minimize function. for a successful fit the error code should be <=2

`xrayutilities.q2ang_fit.`**`exitAngleConst`** (*`angles`*, *`alphaf`*, *`hxrd`*)

helper function for an pseudo-angle constraint for the Q2AngFit-routine.
Parameters

angles: fit parameters of Q2AngFit
alphaf: the exit angle which should be fixed
hxrd: the Experiment object to use for qconversion

xrayutilities.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)

Examples

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

xrayutilities.utilities_noconf module

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

`xrayutilities.utilities_noconf.`**`clear_bit`** (*`f`*, *`offset`*)

clears the bet at an offset

`xrayutilities.utilities_noconf.`**`en2lam`** (*`inp`*)

converts the input energy in eV to a wavelength in Angstrom
Parameters

inp: energy in eV

Returns

float, wavlength in Angstrom

Examples

```
>>> wavelength = en2lam(8048)
```

`xrayutilities.utilities_noconf.`**`energy`** (*`en`*)

convert common energy names to energies in eV
so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1
Parameters

en: energy either as scalar or array with value in eV, which will be returned unchanged; or string with name of emission line

Returns

energy in eV as float

xrayutilities.utilities_noconf.**exchange_filepath** (*orig*, *new*, *keep=0*)
function to exchange the root of a filename with the option of keeping the inner directory structure. This for example includes such a conversion /dir_a/subdir/sample/file.txt -> /home/user/data/sample/file.txt where the innermost directory name is kept (keep=1)
Parameters

orig: original filename which should have its data root replaced

new: new path which should be used instead

keep: (optional) number of inner most directory names which should be kept the same in the output (default = 0). Note that the filename is always return unchanged also with keep=0.

Returns

filename string

Examples

```
>>> exchange_filepath('/dir_a/subdir/sam/file.txt', '/data', 1)
'/data/sam/file.txt'
```

xrayutilities.utilities_noconf.**exchange_path** (*orig*, *new*, *keep=0*)
function to exchange the root of a path with the option of keeping the inner directory structure. This for example includes such a conversion /dir_a/subdir/images/sample -> /home/user/data/images/sample where the two innermost directory names are kept (keep=2)
Parameters

orig: original path which should be replaced by the new path

new: new path which should be used instead

keep: (optional) number of inner most directory names which should be kept the same in the output (default = 0)

Returns

directory path string

Examples

```
>>> exchange_path('/dir_a/subdir/img/sam', '/home/user/data', 2)
'/home/user/data/img/sam'
```

xrayutilities.utilities_noconf.**lam2en** (*inp*)
converts the input wavelength in Angstrom to an energy in eV
Parameters

inp: wavelength in Angstrom

Returns

float, energy in eV

Examples

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

xrayutilities.utilities_noconf.**set_bit** (*f*, *offset*)
sets the bit at an offset

xrayutilities.utilities_noconf.**wavelength** (*wl*)
convert common energy names to energies in eV
so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1
Parameters

wl: wavelength; If scalar or array the wavelength in Angstrom will be returned unchanged, string with emission name is converted to wavelength

Returns

wavelength in Angstrom as float

Module contents

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>

xrayutilities.analysis package

Submodules

xrayutilities.analysis.line_cuts module

`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 extraced scan (bounds=True)

Examples

```
>>> 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*, *ttcenter*, *omrange*, *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

Examples

```
>>> 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 extraced scan (bounds=True)

Examples

```
>>> 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

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)
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

Examples

```
>>> 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

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)

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

Examples

```
>>> 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

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)

qxpos: position at which the line scan should be extracted

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

angrange: integration range in angular 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)

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

wl: wavelength used to determine angular integration positions

Returns

qz,qzint: qz scan coordinates and intensities (bounds=False)

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

Examples

```
>>> 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

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:	om-position at which the radial scan should be extracted
ttcenter:	tt-position at which the radial scan should be extracted
ttrange:	two theta range of the radial scan to extract
npoints:	number of points of the radial scan

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

omrange:	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 two theta positions are returned (default=True)
bounds:	flag to specify if the scan bounds should be returned :(default: False)

Returns

om,tt,radint:	omega,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)

Examples

```
>>> 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

omcenter:	om-position at which the radial scan should be extracted
ttcenter:	tt-position at which the radial scan should be extracted
ttrange:	two theta range of the radial scan to extract
npoints:	number of points of the radial scan

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

omrange:	integration range perpendicular to scan direction
lam:	wavelength for use in the conversion to angular coordinates

Returns

qxrad,qzrad:	reciprocal space boundaries of radial scan

Examples

```
>>>
```

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

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 radial scan should be extracted
qzcenter: qz-position at which the radial scan should be extracted
ttrange: two theta range of the radial scan to extract
npoints: number of points of the radial scan

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

omrange: 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

om,tt,radint: omega,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)

Examples

```
>>> 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

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: om-position at which the 2theta scan should be extracted
ttcenter: tt-position at which the 2theta scan should be extracted
ttrange: two theta range of the scan to extract
npoints: number of points of the radial scan

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

omrange: integration range in omega 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint: two 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)

Examples

```
>>> 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

omcenter:	om-position at which the 2theta scan should be extracted
ttcenter:	tt-position at which the 2theta scan should be extracted
ttrange:	two theta range of the 2theta scan to extract
npoints:	number of points of the 2theta scan

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

omrange:	integration range in omega direction
lam:	wavelength for use in the conversion to angular coordinates

Returns

qxtt,qztt:	reciprocal 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)

Examples

```
>>>
```

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

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 2theta scan should be extracted
qzcenter:	qz-position at which the 2theta scan should be extracted
ttrange:	two theta range of the scan to extract
npoints:	number of points of the radial scan

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

omrange:	integration range in omega 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 two theta positions are returned (default=True)
bounds:	flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint:	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)

Examples

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

xrayutilities.analysis.line_cuts.**getindex** (*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,y:	coordinates of the point of interest (float)
xgrid,ygrid:	grid coordinates in x and y direction (array)

Returns

ix,iy: index of the closest gridpoint (lower left) of the point (x,y)

xrayutilities.analysis.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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

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

xrayutilities.analysis.line_cuts3d.**getindex3d** (*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)

xrayutilities.analysis.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
Parameters

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

Examples

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])

xrayutilities.analysis.sample_align module

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

xrayutilities.analysis.sample_align.**area_detector_calib** (*angle1*, *angle2*, *ccdimages*, *detaxis*, *r_i*, *plot=True*, *cut_off=0.7*, *start=(0*, *0*, *0*, *0)*, *fix=(False*, *False*, *False*, *False)*, *fig=None*, *wl=None*, *plotlog=False*, *nwindow=50*, *debug=False*)
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
angle2: inner detector arm angle
ccdimages: images of the ccd taken at the angles given above
detaxis: detector arm rotation axis :default: ['z+','y-']
r_i: primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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. By default (0,0,0,0) is used.
- **fix:** fix parameters of start (default: (False,False,False,False))
- **fig:** matplotlib figure used for plotting the error :default: None (creates own figure)
- **wl:** wavelength of the experiment in Angstrom (default: config.WAVELENGTH) value does not really matter here but does affect the scaling of the error
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to specify that you want to see verbose output and saving of images to show if the CEN determination works

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*, *False)*, *fig=None*, *plotlog=False*, *nwindow=50*, *debug=False*)

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. Both images from the primary beam hkl = (0,0,0) and from a symmetric reflection hkl = (h,k,l) need to be given for a successful run.

parameters

- **sampleang:** sample 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
- **angle1:** outer detector arm angle
- **angle2:** inner detector arm angle
- **ccdimages:** images of the ccd taken at the angles given above
- **hkls:** array/list of hkl values for every image
- **experiment:** Experiment class object needed to get the UB matrix for the hkl peak treatment
- **material:** material used as reference crystal
- **detaxis:** detector arm rotation axis :default: ['z+','y-']
- **r_i:** primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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: 0.1 = 10%
- **start:** sequence of start values of the fit for parameters, which can not be estimated automatically. these are: tiltazimuth, tilt, detector_rotation, outerangle_offset, sampletilt, sampletiltazimuth, 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))
- **fig:** matplotlib figure used for plotting the error. :default: None (creates own figure)
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to tell if you want to see debug output of the script (switch this to true only if you can handle it :))

xrayutilities.analysis.sample_align.**fit_bragg_peak** (*om*, *tt*, *psd*, *omalign*, *ttalign*, *exphxrd*, *frange=(0.03*, *0.03)*, *peaktype='Gauss'*, *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) or Lorentzian (xrayutilities.math.Lorentz2d)
PLEASE ALWAYS CHECK THE RESULT CAREFULLY!
Parameters

- **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 +/-frangeAA^{-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})
- **peaktype:** can be 'Gauss' or 'Lorentz' to fit either of the two peak shapes
- **plot:** if True (default) function will plot the result of the fit in comparison with the measurement.

Returns

- **Omfit,ttfit,paramss,covariance:** fitted angular values, and the fit parameters (of the Gaussian/Lorentzian) 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)

keyword arguments:

- **r_i:** primary beam direction as vector [xyz][+-]; default: 'y+'
- **detaxis:** detector arm rotation axis [xyz][+-]; default: 'x+'

other options are passed to psd_chdeg function, options include:

plot: flag to specify if a visualization of the fit should be done

usetilt: whether to use model considering a detector tilt, i.e. 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/pixelwidth*pi/180 ~= 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*, *omega0=None*, *plot=True*)

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

phi: azimuths 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.

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.

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

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'*, *mtiltlabel='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*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, i.e. deviation angle of the pixel direction from orthogonal to the primary beam :(default: True)

datap: plot format of data points

modelline: plot format of modelline

modeltilt: plot format of modeltilt

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/pixelwidth*pi/180 = channel/degree for large detector distance with the sample detector disctance 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

Examples

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

Module contents

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.

xrayutilities.io package

Submodules

xrayutilities.io.cbf module

class xrayutilities.io.cbf.**CBFDirectory** (*datapath*, *ext='cbf'*, ***keyargs*)
Bases: **object**
Parses a directory for CBF files, which can be stored to a HDF5 file for further usage

Save2HDF5 (*h5f*, *group=''*, *comp=True*)
Saves the data stored in the CBF 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.
Parameters

h5f: a HDF5 file object or name

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.cbf.**CBFFile** (*fname*, *nxkey='X-Binary-Size-Fastest-Dimension'*, *nykey='X-Binary-Size-Second-Dimension'*, *dtkey='DataType'*, *path=None*)
Bases: **object**

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

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

xrayutilities.io.cbf.**makeNaturalName** (*name*)

xrayutilities.io.desy_tty08 module

class for reading data + header information from tty08 data files

tty08 is a system used at beamline P08 at Hasylab Hamburg and creates simple ASCII files to save the data. Information is easily read from the multicolumn data file. the functions below enable also to parse the information of the header

xrayutilities.io.desy_tty08.**gettty08_scan** (*scanname*, *scannumbers*, **args*, ***keyargs*)
function to obtain the angular cooridinates as well as intensity values saved in TTY08 datafiles. Especially usefull for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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)

**keyargs: keyword arguments are passed on to tty08File

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']).

Examples

```
>>> [om,tt],MAP = xu.io.gettty08_scan('text%05d.dat',36,'omega','gamma')
```

class xrayutilities.io.desy_tty08.**tty08File** (*filename*, *path=None*, *mcadir=None*)

Bases: **object**

Represents a tty08 data file. The file is read during the Constructor call. This class should work for data stored at beamline P08 using the tty08 acquisition system.

Required constructor arguments:

filename: a string with the name of the tty08-file

Optional keyword arguments:

mcadir: directory name of MCA files

Read ()

Read the data from the file

ReadMCA ()

xrayutilities.io.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 (*h5f*, *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.

Parameters

h5f: a HDF5 file object or name

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*, *keep_open=False*)

Bases: **object**

Parse ()

Parse file to find the number of entries and read the respective header information

ReadData (*nimg=0*)

Read the CCD data of the specified image and return the data this function is called automatically when the 'data' property is accessed, but can also be called manually when only a certain image from the file is needed.

Parameters

nimg: number of the image which should be read (starts with 0)

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

data

xrayutilities.io.edf.**makeNaturalName** (*name*)

xrayutilities.io.fastscan module

modules to help with the analysis of FastScan data acquired at the ESRF. FastScan data are X-ray data (various detectors possible) acquired during scanning the sample in real space with a Piezo Scanner. The same functions might be used to analze traditional SPEC mesh scans.

The module provides three core classes:

* FastScan * FastScanCCD * FastScanSeries

where the first two are able to parse single mesh/FastScans when one is interested in data of a single channel detector or are detector and the last one is able to parse full series of such mesh scans with either type of detector

see examples/xrayutilities_kmap_ESRF.py for an example script

class xrayutilities.io.fastscan.**FastScan** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **object**
class to help parsing and treating fast scan data. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source.

grid2D (*nx*, *ny*, ***kwargs*)
function to grid the counter data and return the gridded X,Y and Intensity values.
Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))
gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

motorposition (*motorname*)
read the position of motor with name given by motorname from the data file. In case the motor is included in the data columns the returned object is an array with all the values from the file (although retrace clean is respected if already performed). In the case the motor is not moved during the scan only one value is returned.
Parameters

motorname: name of the motor for which the position is wanted

Returns

val: motor position(s) of motor with name motorname during the scan

parse ()
parse the specfile for the scan number specified in the constructor and store the needed informations in the object properties

retrace_clean ()
function to clean the data of the scan from retrace artifacts created by the zig-zag scanning motion of the piezo actuators the function cleans the xvalues, yvalues and data attribute of the FastScan object.

class xrayutilities.io.fastscan.**FastScanCCD** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **xrayutilities.io.fastscan.FastScan**
class to help parsing and treating fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed

getccdFileTemplate (*specscan*, *datadir=None*, *keepdir=0*, *numfmt='%04d'*)
function to extract the CCD file template string from the comment in the SPEC-file scan-header
Parameters

specscan: spec-scan object from which header the CCD directory should be extracted
datadir: the CCD filenames are usually parsed from the scan object. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.
keepdir: number of directories which should be taken from the specscan. (default: 0)
numfmt: format string for the CCD file number (optional)

Returns

fmtstr: format string for the CCD file name using one number to build the real file name

gridCCD (*nx, ny, ccdnr, roi=None, datadir=None, keepdir=0, nav=[1, 1], gridrange=None, filterfunc=None, imgoffset=0*)
function to grid the internal data and ccd files and return the gridded X,Y and DATA values. DATA represents a 4D with first two dimensions representing X,Y and the remaining two dimensions representing detector channels
Parameters

nx,ny: number of bins in x,y direction
ccdnr: array with ccd file numbers of length length(FastScanCCD.data) OR a string with the data column name for the file ccd-numbers

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

nav: number of detector pixel which will be averaged together (reduces the date size)

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

Returns

X,Y,DATA: regular x,y-grid as well as 4-dimensional data object

class xrayutilities.io.fastscan.**FastScanSeries** (*filenames*, *scannrs*, *nx*, *ny*, **args*, ***kwargs*)

Bases: **object**

class to help parsing and treating a series of fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed.

For the series of FastScans we assume that they are measured at different goniometer angles and therefore transform the data to reciprocal space.

align (*deltax*, *deltay*)

Since a sample drift or shift due to rotation often occurs between different FastScans it should be corrected before combining them. Since determining such a shift is not straight-forward in general the user needs to supply the routine with the shifts in order correct the x,y-values for the different FastScans. Such a routine could for example use the integrated CCD intensities and determine the shift using a cross-convolution.

Parameters

deltax: list of shifts in x-direction for every FastScan in the data structure

deltay: same for the y-direction

getCCDFrames (*posx*, *posy*, *typ='real'*)

function to determine the list of ccd-frame numbers for a specific real space position. The real space position must be within the data limits of the FastScanSeries otherwise an ValueError is thrown

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

Optional:

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

Returns

[[motorpos1, ccdnrs1], [motorpos2, ccdnrs2], ...] where motorposN is

from the N-ths FastScan in the series and ccdnrsN is the list of according CCD-frames

grid2Dall (*nx*, *ny*, ***kwargs*)

function to grid the counter data and return the gridded X,Y and Intensity values from all the FastScanSeries.

Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

gridRSM (*posx, posy, qnx, qny, qnz, qconv, roi=None, nav=[1, 1], typ='real', filterfunc=None, **kwargs*)

function to calculate the reciprocal space map at a certain x,y-position from a series of FastScan measurements it is necessary to specify the number of grid-oints for the reciprocal space map and the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qnx: number of points in the Qx direction of the gridded reciprocal space map

qny: same for y direction

qnz: same for z directino

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

Returns

Gridder3D object with gridded reciprocal space map

rawRSM (*posx, posy, qconv, roi=None, nav=[1, 1], typ='real', datadir=None, keepdir=0, filterfunc=None, **kwargs*)

function to return the reciprocal space map data at a certain x,y-position from a series of FastScan measurements. It necessary to give the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

Returns

Qx,qy,qz,ccddata,valuelist: raw data of the reciprocal space map and valuelist containing the ccdframe numbers and corresponding motor positions

read_motors ()
read motor values from the series of fast scans

retrace_clean ()
perform retrace clean for every FastScan in the series

xrayutilities.io.helper module

convenience functions to open files for various data file reader

these functions should be used in new parsers since they transparently allow to open gzipped and bzipped files

class xrayutilities.io.helper.**xu_h5open** (*f*, *mode='r'*)
Bases: **object**
helper object to decide if a HDF5 file has to be opened/closed when using with a 'with' statement.

xrayutilities.io.helper.**xu_open** (*filename*, *mode='rb'*)
function to open a file no matter if zipped or not. Files with extension '.gz' or '.bz2' are assumed to be compressed and transparently opened to read like usual files.
Parameters

filename: filename of the file to open (full including path)

mode: mode in which the file should be opened

Returns

file handle of the opened file

If the file does not exist an IOError is raised by the open routine, which is not caught within the function

xrayutilities.io.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 with

1. RoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point.
2. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

readImage (*filename*, *path=None*)
read image file and correct for dark- and flatfield in case the necessary data are available.
returned data = ((image data)-(darkfield))/flatfield*average(flatfield)
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed. supported extensions: .tif, .bin and .bin.xz

class xrayutilities.io.imagereader.**PerkinElmer** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse PerkinElmer CCD frames (*.tif) 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.**Pilatus100K** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse Dectris Pilatus 100k frames (*.tiff) to numpy arrays Ignore the header since it seems to contain no useful data

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.

class xrayutilities.io.imagereader.**TIFFRead** (*filename*, *path=None*)
Bases: **xrayutilities.io.imagereader.ImageReader**
class to Parse a TIFF file including extraction of information from the file header in order to determine the image size and data type
The data stored in the image are available in the 'data' property.

xrayutilities.io.imagereader.**get_tiff** (*filename*, *path=None*)
read tiff image file and return the data
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed.

xrayutilities.io.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*, *path=''*)
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*, *namespace=''*)

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.XRDMLFile class is used. The function can be used for parsing maps measured with the PIXCel 1D detector (and in limited way also for data acquired with a point detector -> see getxrdml_scan instead).
Parameters

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 usefull!

Returns

om,tt,psd: as flattened numpy arrays

Examples

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

xrayutilities.io.panalytical_xml.**getxrdml_scan** (*filetemplate*, **motors*, ***kwargs*)
parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLFile class is used. The function can be used for parsing arbitrary scans and will return the the motor values of the scan motor and additionally the positions of the motors given by in the "*motors" argument
Parameters

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

***motors: motor names to return: e.g.: 'Omega','2Theta',...**

one can also use abbreviations 'Omega' = 'om' = 'o' '2Theta' = 'tt' = 't' 'Chi' = 'c' 'Phi' = 'p'

****kwargs:**

scannrs: int or list of scan numbers
path: common path to the filenames

Returns

scanmot,mot1,mot2,...,detectorint: as flattened numpy arrays

Examples

```
>>> scanmot,om,tt,inte = xrayutilities.io.getxrdml_scan(
        "samplename_1.xrdml", 'om', 'tt', path="./data")
```

xrayutilities.io.pdcif module

class xrayutilities.io.pdcif.**pdCIF** (*filename*, *datacolumn=None*)
Bases: `object`
the class implements a primitive parser for pdCIF-like files. It reads every entry and collects the information in the header attribute. The first loop containing one of the intensity fields is assumed to be the data the user is interested in and is transfered to the data array which is stored as numpy record array the columns can be accessed by name

intensity fields:

_pd_meas_counts_total, _pd_meas_intensity_total, _pd_proc_intensity_total, _pd_proc_intensity_net, _pd_calc_intensity_total, _pd_calc_intensity_net
alternatively the data column name can be given as argument to the constructor

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

class xrayutilities.io.pdcif.**pdESG** (*filename*, *datacolumn=None*)
Bases: **xrayutilities.io.pdcif.pdCIF**
class for parsing multiple pdCIF loops in one file. This includes especially *.esg files which are supposed to consist of multiple loops of pdCIF data with equal length.
Upon parsing the class tries to combine the data of these different scans into a single data matrix -> same shape of subscan data is assumed

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

xrayutilities.io.pdcif.**remove_comments** (*line*, *sep='#'*)

xrayutilities.io.rigaku_ras module

class for reading data + header information from Rigaku RAS (3-column ASCII) files

Such datafiles are generated by the Smartlab Guidance software from Rigaku.

class xrayutilities.io.rigaku_ras.**RASFile** (*filename*, *path=None*)
Bases: **object**
Represents a RAS data file. The file is read during the constructor call
Required constructor arguments:

filename: a string with the name of the ras-file

keyword argument (optional):

path: path to the data file

Read ()
Read the data from the file

class xrayutilities.io.rigaku_ras.**RASScan** (*filename*, *pos*)
Bases: **object**
Represents a single Scan portion of a RAS data file. The scan is parsed during the constructor call
Required constructor arguments:

filename: file name of the data file
pos: seek position of the RAS_HEADER_START line

xrayutilities.io.rigaku_ras.**getras_scan** (*scanname*, *scannumbers*, **args*, ***kwargs*)
function to obtain the angular cooridinates as well as intensity values saved in RAS datafiles. Especially useful for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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: keyword arguments forwarded to RASFile function

Returns

rasdata

or

[ang1,ang2,...],rasdata:

angular positions are extracted from the respective scan header together with all the data values as stored in the data file (includes the intensities e.g. rasdata['int']).

Examples

```
>>> [om,tt],MAP = xu.io.getras_scan('text%05d.ras',36,'Omega','TwoTheta')
```

xrayutilities.io.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

xrayutilities.io.seifert module

a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two posibilities 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**

helper class to represent a Seifert (NJA) scan file header

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

Bases: **object**

Class to parse a Seifert (NJA) multiscan file

parse ()

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

Bases: **object**

Class to parse a single Seifert (NJA) scan file

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.

Parameters

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: can be either "map" (reciprocal space map measured with a regular Seifert job (default)) or "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

Examples

```
>>> 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 preceeding _.

xrayutilities.io.spec module

a 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**

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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

comp: activate 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**

class to parse a SPEC log file to find the command history

Parse ()

class xrayutilities.io.spec.**SPECScan** (*name*, *scannr*, *command*, *date*, *time*, *itime*, *colnames*, *hoffset*, *doffset*, *fname*, *imopnames*, *imopvalues*, *scan_status*)

Bases: **object**

Represents a single SPEC scan. This class is usually not called by the user directly but used via the SPECFile class.

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=''*, *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 ususally 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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

group: name or group object of the HDF5 group where to store the data

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

optattrs: a dictionary with optional attributes to store for the data

comp: activate 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 aguments:

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*, ***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:**

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 cooridinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially useful 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 h5py 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 ommited the first child node of h5f.root will be used

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

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']).

Examples

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

xrayutilities.io.spec.**getspec_scan** (*specf*, *scans*, **args*, ***kwargs*)

function to obtain the angular cooridinates as well as intensity values saved in a SPECFile. Especially useful to combine the data from multiple scans.
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

specf: SPECFile object

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

args: names of the motors and counters (strings)

keyword arguments:

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

Returns

[ang1,ang2,...]:

coordinates and counters from the SPEC file

Examples

```
>>> [om, tt, cnt2] = xu.io.getspec_scan(s, 36, 'omega', 'gamma',
                                        'Counter2')
```

xrayutilities.io.spec.**makeNaturalName** (*name*)

xrayutilities.io.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='/'*, *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

name: name of the group where to store the data

optional keyword arguments:

group: root group where to store the data

mcaname: Name of the MCA in the HDF5 file

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**

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

h5f: file object of a HDF5 file opened using h5py

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

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

omname: name of the omega motor (or its equivalent)

ttname: name of the two theta motor (or its equivalent)

****kwargs (optional):**

mca: name 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']).

Module contents

xrayutilities.materials package

Submodules

xrayutilities.materials.atom module

module containing the Atom class which handles the database access for atomic scattering factors and the atomic mass.

class xrayutilities.materials.atom.**Atom** (*name*, *num*)

Bases: **object**

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

function to calculate the atomic structure factor F

Parameters

q: momentum transfer

en: 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'*)

weight

xrayutilities.materials.cif module

class xrayutilities.materials.cif.**CIFFile** (*filename*, *digits=3*)

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.

xrayutilities.materials.database module

module to handle the access to the optical parameters database

class xrayutilities.materials.database.**DataBase** (*fname*)
Bases: **object**

Close ()
Close an opend 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*, *dset='default'*)
Obtain the f0 scattering factor component for a particular momentum transfer q.

required input argument:

q: single float value or numpy array
dset: specifies which dataset (different oxidation states) should be used

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*, *subset='default'*)
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
subset: specifies under which name the f0 values should be saved

SetF1F2 (*en*, *f1*, *f2*)
Set f1, f2 values for the active material.

required input arguments:

en: list or numpy array with energy in (eV)
f1: list or numpy array with f1 values
f2: list 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:

name: string with the name of the material

SetWeight (*weight*)
Save weight of the element as float

required input argument:

weight: atomic standard weight of the element (float)

xrayutilities.materials.database.**add_f0_from_intertab** (*db*, *itf*)
Read f0 data from International Tables of Crystallography and add it to the database.

xrayutilities.materials.database.**add_f0_from_xop** (*db*, *xop*)
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*, *hf*)
Read f1 and f2 data from Henke database and add it to the database.

xrayutilities.materials.database.**add_f1f2_from_kissel** (*db*, *kf*)
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. The mass of the natural isotope mixture is taken from the NIST data!

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

xrayutilities.materials.elements module

xrayutilities.materials.lattice module

module handling crystal lattice structures. A Lattice consists of unit cell parameters and a LatticeBase. It offers methods to calculate the reciprocal space position of Bragg peaks and their structure factor.

xrayutilities.materials.lattice.**AlGaAsLattice** (*aal*, *aga*, *aas*, *a*, *x*)

xrayutilities.materials.lattice.**BCCLattice** (*aa*, *a*)

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

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

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

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

xrayutilities.materials.lattice.**CubicLattice** (*a*, *base=None*)

Returns a Lattice object representing a cubic lattice.

Parameters

a: lattice parameter

base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

xrayutilities.materials.lattice.**DiamondLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCSharedLattice** (*aa*, *ab*, *occa*, *occb*, *a*)

xrayutilities.materials.lattice.**GeTeRhombohedral** (*aa*, *ab*, *a*, *ang*, *x=0.237*)

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*)

xrayutilities.materials.lattice.**HexagonalLattice** (*a*, *c*, *base=None*)

Returns a Lattice object representing a hexagonal lattice.

Parameters

a: lattice parameter a

c: lattice parameter c

base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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 and unit cell defined by three vectors.

ApplyStrain (*eps*)

Applies a certain strain on a lattice. The result is a change in the base vectors. The full strain matrix (3x3) needs to be given. .. note:: Note: NO elastic response of the material will be considered!

requiered input arguments:

eps: a 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 (angstrom^3)

a

a1

a2

a3

alpha

b

beta

c

gamma

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
Parameters

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*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.**MagnetiteLattice** (*aa*, *ab*, *ac*, *a*, *x=0.255*)

xrayutilities.materials.lattice.**MonoclinicLattice** (*a*, *b*, *c*, *beta*, *base=None*)
Returns a Lattice object representing a hexagonal lattice.
Parameters

a: lattice parameter a
b: lattice parameter b
c: lattice parameter c
beta: monoclinic unit cell angle beta (deg)
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

xrayutilities.materials.lattice.**NiAsLattice** (*aa*, *ab*, *a*, *c*, *biso=0.0*)

xrayutilities.materials.lattice.**OrthorhombicLattice** (*a*, *b*, *c*, *base=None*)
Returns a Lattice object representing a tetragonal lattice.
Parameters

a: lattice parameter a
b: lattice parameter b
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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*)
creates the primitive unit cell of a RockSalt structure. For the more commonly used cubic reprentation see RockSalt_Cubic_Lattice

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

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

xrayutilities.materials.lattice.**SiGeLattice** (*asi*, *age*, *a*, *xge*)

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

xrayutilities.materials.lattice.**TetragonalLattice** (*a*, *c*, *base=None*)
Returns a Lattice object representing a tetragonal lattice.
Parameters

a: lattice parameter a
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

xrayutilities.materials.lattice.**TriclinicLattice** (*a*, *b*, *c*, *alpha*, *beta*, *gamma*, *base=None*)

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*)

xrayutilities.materials.material module

Classes decribing materials. Materials are devided with respect to their crystalline state in either Amorphous or Crystal types. While for most materials their crystalline state is defined few materials are also included as amorphous which can be useful for calculation of their optical properties.

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

RelaxationTriangle (*hkl*, *sub*, *exp*)
function which returns the relaxation trianlge for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class
Parameters

hkl: Miller Indices
sub: substrate material or lattice constant (Instance of Crystal 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

class xrayutilities.materials.material.**Amorphous** (*name*, *density*, *atoms=None*, *cij=None*)
Bases: **xrayutilities.materials.material.Material**
amorphous materials are described by this class

beta (*en='config'*)
function to calculate the imaginary part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

delta (*en='config'*)
function to calculate the real part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

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.**Crystal** (*name*, *lat*, *cij=None*, *thetaDebye=None*)
Bases: **xrayutilities.materials.material.Material**
Crystalline materials are described by this class

ApplyStrain (*strain*)

Applies a certain strain on the lattice of the material. The result is a change in the base vectors of the real space as well as reciprocal space lattice. The full strain matrix (3x3) needs to be given. Note: NO elastic response of the material will be considered!

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.
Parameters

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
Parameters

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
Parameters

q0: vectorial momentum transfer (vectors as list,tuple or numpy array are valid)
en: list, tuple or array of energy values in eV
temp: temperature 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
Parameters

q: vectorial 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)])
en0: energy value in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature 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)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 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
Parameters

q: momentum transfer in (1/A)
en: xray energy in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature used for Debye-Waller-factor calculation
polarization: either 'S' (default) sigma or 'P' pi polarization

Returns

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

dTheta (*Q*, *en='config'*)
function to calculate the refractive peak shift
Parameters

Q: momentum transfer (1/A)
en: x-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaTheta: peak 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)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

density
calculates the mass density of an material from the mass of the atoms in the unit cell.
Returns
mass density in kg/m^3

distances ()
function to obtain distances of atoms in the crystal up to the unit cell size (largest value of a,b,c is the cut-off)
returns a list of tuples with distance d and number of occurence n [(d1,n1),(d2,n2),...]

Note

Note: if the base of the material is empty the list will be empty

environment (*pos, **kwargs)

Returns a list of neighboring atoms for a given position within the the unit cell.

Parameters

pos: list or numpy array with the fractional coordinated in the unit cell

keyword arguments:

maxdist: maximum distance wanted in the list of neighbors :(default: 7)

Returns

list of tuples with (distance,atomType,multiplicity) giving distance (sorted) and type of neighboring atoms together with the amount of atoms at the given distance

classmethod **fromCIF** (*ciffilename*)

Create a Crystal from a CIF file. Name and

Parameters

ciffilename: filename of the CIF file

Returns

Crystal instance

planeDistance (*hkl)

determines the lattice plane spacing for the planes specified by (hkl)

Parameters

h,k,l: Miller indices of the lattice planes given either as list,tuple or seperate arguments

Returns

d: the lattice plane spacing as float

Examples

```
>>> xu.materials.Si.planeDistance(0,0,4)
1.3577600000000001
```

or

```
>>> xu.materials.Si.planeDistance((1,1,1))
3.1356124059796255
```

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

Parameters

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 symetric peak. As an additional input the substrates lattice parameter and the degree of relaxation must be given
Parameters

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
Parameters

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'*, *base=None*)
general material with primitive unit cell but possibility for different a,b,c and alpha,beta,gamma
Parameters

a,b,c: unit cell extenstions (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
base: instance of LatticeBase

returns a Crystal 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
Parameters

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*, *cij=None*)
Bases: **object**
base class for all Materials. common properties of amorphous and crystalline materials are described by this class from which Amorphous and Crystal are derived from.

beta (*en='config'*)

chi0 (*en='config'*)
calculates the complex chi_0 values often needed in simulations. They are closely related to delta and beta (n = 1 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

critical_angle (*en='config'*, *deg=True*)
calculate critical angle for total external reflection

Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

deg: return angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

delta (*en='config'*)

density

idx_refraction (*en='config'*)

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

Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

xrayutilities.materials.material.**PseudomorphicMaterial** (*sub*, *layer*, *relaxation=0*, *trans=None*)

This function returns a material whos lattice is pseudomorphic on a particular substrate material. The two materials must have similar unit cell definitions for the algorithm to work correctly, i.e. it does not work for combiniations of materials with different lattice symmetry.

Parameters

sub: substrate material

layer: bulk material of the layer

relaxation: degree of relaxation 0: pseudomorphic, 1: relaxed :(default: 0)

trans: Transformation which transforms lattice directions into a surface orientated coordinate frame (x,y inplane, z out of plane). If None a (001) surface geometry of a cubic material is assumed.

Returns

An instance of Crystal holding the new pseudomorphically strained material.

xrayutilities.materials.material.**WZTensorFromCub** (*c11ZB*, *c12ZB*, *c44ZB*)

Determines the hexagonal elastic tensor from the values of the cubic elastic tensor under the assumptions presented in Phys. Rev. B 6, 4546 (1972), which are valid for the WZ <-> ZB polymorphs.

Parameters

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

Returns

6x6 matrix with elastic constants

Implementation according to a patch submitted by Julian Stangl

xrayutilities.materials.material.**index_map_ij2ijkl** (*ij*)

xrayutilities.materials.material.**index_map_ijkl2ij** (*i*, *j*)

xrayutilities.materials.predefined_materials module

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

Bases: **xrayutilities.materials.material.CubicAlloy**

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

Module contents

xrayutilities.math package

Submodules

xrayutilities.math.algebra module

module providing analytic algebraic functions not implemented in scipy or any other dependency of xrayutilities. In particular the analytic solution of a quartic equation which is needed for the solution of the dynamic scattering equations.

xrayutilities.math.algebra.**solve_quartic** (*a4*, *a3*, *a2*, *a1*, *a0*)
analytic solution [1] of the general quartic equation. The solved equation takes the form:
a4*z**4 + a3*z**3 + a2*z**2 + a1*z + a0
Returns

tuple of the four (complex) solutions of aboves equation.

[1] http://mathworld.wolfram.com/QuarticEquation.html

xrayutilities.math.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,y:	data coordinates (do NOT need to be regularly spaced)
data:	data set used for fitting (e.g. intensity at the data coords)
start:	set of starting parameters for the fit used as first parameter of function fit_function
drange:	limits 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_function:	function 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=300*)
Gauss fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting
Parameters

xdata:	xcoordinates of the data to be fitted
ydata:	ycoordinates of the data which should be fit

keyword parameters:

iparams:	initial paramters for the fit, determined automatically if not given

maxit: maximal 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

`xrayutilities.math.fit.`**`linregress`** (*x*, *y*)
fast linregress to avoid usage of scipy.stats which is slow!
Parameters

x,y: data coordinates and values

Returns

p, rsq: parameters of the linear fit (slope, offest) and the R^2 value
Examples

```
>>> (k, d), R2 = xu.math.linregress(x, y)
```

`xrayutilities.math.fit.`**`multGaussFit`** (*`*args`*, *`**kwargs`*)
convenience function to keep API stable see multPeakFit for documentation

`xrayutilities.math.fit.`**`multGaussPlot`** (*`*args`*, *`**kwargs`*)
convenience function to keep API stable see multPeakPlot for documentation

`xrayutilities.math.fit.`**`multPeakFit`** (*x*, *`data`*, *`peakpos`*, *`peakwidth`*, *`dranges=None`*, *`peaktype='Gaussian'`*)
function to fit multiple Gaussian/Lorentzian peaks with linear background to a set of data
Parameters

x: x-coordinate of the data
data: data array with same length as x
peakpos: initial parameters for the peak positions
peakwidth: initial values for the peak width
dranges: list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as peakpos
peaktype: type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'

Returns

pos,sigma,amp,background

Pos: list of peak positions derived by the fit
Sigma: list of peak width derived by the fit
Amp: list of amplitudes of the peaks derived by the fit
Background: array of background values at positions x

`xrayutilities.math.fit.`**`multPeakPlot`** (*x*, *`fpos`*, *`fwidth`*, *`famp`*, *`background`*, *`dranges=None`*, *`peaktype='Gaussian'`*, *`fig='xu_plot'`*, *`fact=1.0`*)
function to plot multiple Gaussian/Lorentz peaks with background values given by an array
Parameters

x: x-coordinate of the data
fpos: list of positions of the peaks
fwidth: list of width of the peaks
famp: list of amplitudes of the peaks
background: array with background values
dranges: list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as fpos
peaktype: type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'
fig: matplotlib figure number or name

fact: factor to use as multiplicator in the plot

`xrayutilities.math.fit.`**`peak_fit`** (*xdata*, *ydata*, *iparams=[*, *]*, *peaktype='Gauss'*, *maxit=300*, *background='constant'*, *plot=False*, *func_out=False*, *debug=False*)

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

Parameters

xdata: xcoordinates of the data to be fitted

ydata: ycoordinates of the data which should be fit

keyword parameters:

iparams: initial paramters for the fit, determined automatically if not specified

peaktype: type of peak to fit: 'Gauss', 'Lorentz', 'PseudoVoigt', 'PseudoVoigtAsym'

maxit: maximal iteration number of the fit

background: type of background, either 'constant' or 'linear'

plot: flag to ask for a plot to visually judge the fit. If plot is a string it will be used as figure name, which makes reusing the figures easier.

func_out: returns the fitted function, which takes the independent variables as only argument (f(x))

Returns

params,sd_params,itlim[,fitfunc]

the parameters as defined in function Gauss1d/Lorentz1d/PseudoVoigt1d/ PseudoVoigt1dasym(x, *param). In the case of linear background one more parameter is included! For every parameter the corresponding errors of the fit 'sd_params' are returned. A boolean flag 'itlim', which is False in the case of a successful fit is added by default. Further the function used in the fit can be returned (see func_out).

xrayutilities.math.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

Examples

Calling with a list of parameters needs a call looking as shown below (note the '*') or explicit listing of the parameters: >>> Gauss1d(x,*p) >>> Gauss1d(numpy.linspace(0,10,100), 5, 1, 1e3, 0)

`xrayutilities.math.functions.`**`Gauss1dArea`** (**p*)

function to calculate the area of a Gauss function with neglected background

Parameters

p: list of parameters of the Gauss-function [XCEN,SIGMA,AMP,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

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.**Gauss2dArea** (**p*)
function to calculate the area of a 2D Gauss function with neglected background
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,ANGLE,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

xrayutilities.math.functions.**Gauss3d** (*x*, *y*, *z*, **p*)
function to calculate a general three dimensional Gaussian
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,ZCEN,SIGMAX,SIGMAY,SIGMAZ,AMP,BACKGROUND] SIGMA = FWHM / (2*sqrt(2*log(2)))

x,y,z: coordinate(s) where the function should be evaluated

Returns
the value of the Gaussian described by the parameters p at positions (x,y,z)

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: 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.**Lorentz1dArea** (**p*)
function to calculate the area of a Lorentz function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

Returns
the area of the Lorentzian described by the parameters p

xrayutilities.math.functions.**Lorentz1d_der_p** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect the parameters p
for parameter description see Lorentz1d

xrayutilities.math.functions.**Lorentz1d_der_x** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect to x
for parameter description see Lorentz1d

xrayutilities.math.functions.**Lorentz2d** (*x*, *y*, **p*)
function to calculate a general two dimensional Lorentzian
Parameters

p: list 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,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.**NormGauss1d** (*x*, **p*)
function to calculate a normalized one dimensional Gaussian
Parameters

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

x: coordinate(s) where the function should be evaluated

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

xrayutilities.math.functions.**PseudoVoigt1d** (*x*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

xrayutilities.math.functions.**PseudoVoigt1dArea** (**p*)
function to calculate the area of a pseudo Voigt function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the area of the PseudoVoigt described by the parameters p

xrayutilities.math.functions.**PseudoVoigt1d_der_p** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect the parameters p
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1d_der_x** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect to x
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1dasym** (*x*, **p*)
function to calculate an asymmetric pseudo Voigt function as linear combination of asymmetric Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHMLEFT,FWHMRIGHT,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

`xrayutilities.math.functions.`**`PseudoVoigt2d`** (*x*, *y*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak in two dimensions
Parameters

x,y: coordinate(s) where the function should be evaluated

p: list of parameters of the pseudo Voigt-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the value of the PseudoVoigt 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

p: list of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2, SIGMAX2,SIGMAY2,AMP2,ANGLE2,BACKGROUND] 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.`**`heaviside`** (*x*)
Heaviside step function for numpy arrays
Parameters

x: any scalar of ndarray object

Returns

s: Heaviside step function evaluated for all values of x

`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

data: 1d numpy array with experimental data

threshold: threshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.`**`multPeak1d`** (*x*, **args*)
function to calculate the sum of multiple peaks in 1D. the peaks can be of different type and a background function (polynom) can also be included.
Parameters

x: coordinate where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'a': asym. PseudoVoigt, 'p': polynom the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss1d, math.Lorentz1d, math.PseudoVoigt1d, math.PseudoVoigt1dasym, and numpy.polyval for details of the different function types.

Returns

value of the sum of functions at position x

`xrayutilities.math.functions.`**`multPeak2d`** (*x*, *y*, **args*)

function to calculate the sum of multiple peaks in 2D. the peaks can be of different type and a background function (polynom) can also be included.

Parameters

x,y: coordinates where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'c': constant the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss2d, math.Lorentz2d, math.PseudoVoigt2d for details of the different function types. The constant accepts a single float which will be added to the data

Returns

value of the sum of functions at position (x,y)

`xrayutilities.math.functions.`**`smooth`** (*x*, *n*)

function to smooth an array of data by averaging N adjacent data points

Parameters

x: 1D data array

n: number of data points to average

Returns

xsmooth: smoothed array with same length as x

xrayutilities.math.misc module

`xrayutilities.math.misc.`**`center_of_mass`** (*pos*, *data*, *background='none'*, *full_output=False*)

function to determine the center of mass of an array

Parameters

pos: position of the data points

data: data values

background: type of background, either 'none', 'constant' or 'linear'

full_output: return background cleaned data and background-parameters

Returns

center of mass position (single float)

`xrayutilities.math.misc.`**`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)

Parameters

pos: position of the data points

data: data values

Returns

fwhm value (single float)

xrayutilities.math.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.

class xrayutilities.math.transforms.**AxisToZ_keepXY** (*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/y-axis of the new coordinate frame is created to be similar to the old x and y directions. This variant of AxisToZ assumes that the new Z-axis has its main component along the Z-direction

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*, *rank=1*)
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 size of the transformation matrix.

rank: rank of the supplied object. allowed values are 1, 2, and 4

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 radiants.

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 radiants.

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 radiants.

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
Parameters

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

Examples

```
>>> 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

xrayutilities.math.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)*norm(v2)*cos(alpha*)

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 radiants

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

Module contents

xrayutilities.simpack package

Submodules

xrayutilities.simpack.fit module

`xrayutilities.simpack.fit.`**`fit_xrr`** (*reflmod*, *params*, *ai*, *data=None*, *eps=None*, *xmin=-inf*, *xmax=inf*, *plot=False*, *verbose=False*, *elog=True*, *maxfev=500*)

optimize function for a Reflectivity Model using lmfit. The fitting parameters must be specified as instance of lmfits Parameters class.

Parameters

reflmod: preconfigured SpecularReflectivityModel

params: instance of lmfits Parameters class. For every layer the parameters '{}_thickness', '{}_roughness', '{}_density', with '{}' representing the layer name are supported. In addition the setup parameters: - 'I0' primary beam intensity - 'background' background added to the simulation - 'sample_width' size of the sample along the beam - 'beam_width' width of the beam in the same units - 'resolution_width' width of the resolution function in deg - 'shift' experimental shift of the incidence angle array

ai: array of incidence angles for the calculation

data: experimental data which should be fitted

eps: (optional) error bar of the data

xmin: minimum value of ai which should be used. a mask is generated to cut away other data

xmax: maximum value of ai which should be used. a mask is generated to cut away other data

plot: flag to decide wheter an plot should be created showing the fit's progress. If plot is a string it will be used as figure name, which makes reusing the figures easier.

verbose: flag to tell if the variation of the fitting error should be output during the fit.

elog: logarithmic error during the fit

maxfev: maximum number of function evaluations during the leastsq optimization

Returns

res: MinimizerResult object from lmfit, which contains the fitted parameters in res.params (see res.params.pretty_print) or try lmfit.report_fit(res)

xrayutilities.simpack.models module

class xrayutilities.simpack.models.**DynamicalModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.SimpleDynamicalCoplanarModel**

Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a generalized 2-beam theory (4 tiepoints, S and P polarizations)

The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*)

performs the actual diffraction calculation for the specified incidence angles and uses an analytic solution for the quartic dispersion equation

Parameters

alphai: vector of incidence angles (deg)

hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)

geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**KinematicalModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.LayerModel**

Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of one (hkl) Bragg peak, however considers the variation of the structure factor for different 'q'. The surface geometry is specified using the Experiment-object given to the constructor.

init_chi0 ()

calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness does NOT require this!)

simulate (*qz*, *hkl*, *absorption=False*, *refraction=False*)

performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a single Bragg peak.

Parameters

qz: simulation positions along qz

hkl: Miller indices of the Bragg peak whos truncation rod should be calculated

absorption: flag to tell if absorption correction should be used

refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**KinematicalMultiBeamModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.KinematicalModel**
Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of several Bragg peaks on the truncation rod and considers the variation of the structure factor. In order to use a analytical description for the kinematic diffraction signal all layer thicknesses are changed to a multiple of the respective lattice parameter along qz. Therefore this description only works for (001) surfaces.

simulate (*qz*, *hkl*, *absorption=False*, *refraction=True*)
performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a full truncation rod
Parameters

qz: simulation positions along qz
hkl: Miller indices of the Bragg peak whos truncation rod should be calculated
absorption: flag to tell if absorption correction should be used
refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**LayerModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.Model**
generic model class from which further thin film models can be derived from

class xrayutilities.simpack.models.**Model** (*experiment*, ***kwargs*)
Bases: **object**
generic model class from which further models can be derived from

convolute_resolution (*x*, *y*)
convolve simulation result with a Gaussian resolution function
Parameters

x: x-values of the simulation, units of x also decide about the unit of the resolution_width parameter
y: y-values of the simulation

Returns

convoluted y-data with same shape as y

scale_simulation (*y*)
scale simulation result with primary beam flux/intensity and add a background.
Parameters

y: y-values of the simulation

Returns

scaled y values

class xrayutilities.simpack.models.**SimpleDynamicalCoplanarModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.KinematicalModel**
Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a simplified 2-beam theory (2 tiepoints, S and P polarizations)
No restrictions are made for the surface orientation.
The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

> ***Note***
>
> Note: This model should not be used in real life scenarios since the made approximations severely fail for distances far from the reference position.

get_polarizations ()
return list of polarizations which should be calculated

join_polarizations (*Is*, *Ip*)
method to calculate the total diffracted intensity from the intensities of S and P-polarization.

set_hkl (hkl*)**
To speed up future calculations of the same Bragg peak optical parameters can be pre-calculated using this function.
Parameters

hkl: Miller indices of the Bragg peak for the calculation

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*, *idxref=1*)
performs the actual diffraction calculation for the specified incidence angles.
Parameters

alphai: vector of incidence angles (deg)
hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)
geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence
idxref: index of the reference layer. In order to get accurate peak position of the film peak you want this to be the index of the film peak (default: 1). For the substrate use 0.

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**SpecularReflectivityModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.LayerModel**
model for specular reflectivity calculations

densityprofile (*nz*, *plot=False*)
calculates the electron density of the layerstack from the thickness and roughness of the individual layers
Parameters

nz: number of values on which the profile should be calculated
plot: flag to tell if a plot of the profile should be created

Returns

z, eprof: coordinates and electron profile. z = 0 corresponds to the
surface

init_cd ()
calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness and roughness do NOT require this!)

simulate (*alphai*)
performs the actual reflectivity calculation for the specified incidence angles
Parameters

alphai: vector of incidence angles

Returns

vector of intensities of the reflectivity signal

xrayutilities.simpack.models.**startdelta** (*start*, *delta*, *num*)

xrayutilities.simpack.smaterials module

class xrayutilities.simpack.smaterials.**CrystalStack** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.LayerStack**
extends the built in list type to enable building a stack of crystalline Layers by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**GradedLayerStack** (*alloy*, *xfrom*, *xto*, *nsteps*, *thickness*, ***kwargs*)
Bases: **xrayutilities.simpack.smaterials.CrystalStack**
generates a sequence of layers with a gradient in chemical composition

class xrayutilities.simpack.smaterials.**Layer** (*material*, *thickness*, ***kwargs*)
Bases: **xrayutilities.simpack.smaterials.SMaterial**
Object describing part of a thin film sample. The properties of a layer :are:

Material: an xrayutilties material describing optical and crystal properties of the thin film
Thickness: film thickness in Angstrom
Roughness: root mean square roughness of the top interface in Angstrom

class xrayutilities.simpack.smaterials.**LayerStack** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.MaterialList**
extends the built in list type to enable building a stack of Layer by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**MaterialList** (*name*, **args*)
Bases: **_abcoll.MutableSequence**
class representing the basics of a list of materials for simulations within xrayutilities. It extends the built in list type.

check (*v*)

insert (*i*, *v*)

class xrayutilities.simpack.smaterials.**PseudomorphicStack001** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.CrystalStack**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 001 and materials must be cubic/tetragonal.

insert (*i*, *v*)

make_epitaxial (*i*)

trans = *<xrayutilities.math.transforms.Transform object at 0x7f2db1e4ae50>*

class xrayutilities.simpack.smaterials.**PseudomorphicStack111** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.PseudomorphicStack001**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 111 and materials must be cubic.

trans = *<xrayutilities.math.transforms.CoordinateTransform object at 0x7f2db0fe3090>*

class xrayutilities.simpack.smaterials.**SMaterial** (*material*, ***kwargs*)
Bases: **object**
Simulation Material. Extends the xrayutilities Materials by properties needed for simulations

Module contents

simulation subpackage of xrayutilities.

This package provides possibilities to simulate X-ray diffraction and reflectivity curves of thin film samples. It could be extended for more general use in future if there is demand for that.

In addition it provides a fitting routine for reflectivity data which is based on lmfit.

xrayutilities

xrayutilities package

Subpackages

xrayutilities.analysis package

Submodules

xrayutilities.analysis.line_cuts module

`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 extraced scan (bounds=True)

Examples

```
>>> 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*, *ttcenter*, *omrange*, *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

Examples

```
>>> 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 extraced scan (bounds=True)

Examples

```
>>> 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

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)
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

Examples

```
>>> 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

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)

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

Examples

```
>>> 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

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)

qxpos: position at which the line scan should be extracted

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

angrange: integration range in angular 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)

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

wl: wavelength used to determine angular integration positions

Returns

qz,qzint: qz scan coordinates and intensities (bounds=False)

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

Examples

```
>>> 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

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:	om-position at which the radial scan should be extracted
ttcenter:	tt-position at which the radial scan should be extracted
ttrange:	two theta range of the radial scan to extract
npoints:	number of points of the radial scan

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

omrange:	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 two theta positions are returned (default=True)
bounds:	flag to specify if the scan bounds should be returned :(default: False)

Returns

om,tt,radint:	omega,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)

Examples

```
>>> 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

omcenter:	om-position at which the radial scan should be extracted
ttcenter:	tt-position at which the radial scan should be extracted
ttrange:	two theta range of the radial scan to extract
npoints:	number of points of the radial scan

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

omrange:	integration range perpendicular to scan direction
lam:	wavelength for use in the conversion to angular coordinates

Returns

qxrad,qzrad:	reciprocal space boundaries of radial scan

Examples

```
>>>
```

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

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 radial scan should be extracted
qzcenter: qz-position at which the radial scan should be extracted
ttrange: two theta range of the radial scan to extract
npoints: number of points of the radial scan

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

omrange: 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

om,tt,radint: omega,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)

Examples

```
>>> 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

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: om-position at which the 2theta scan should be extracted
ttcenter: tt-position at which the 2theta scan should be extracted
ttrange: two theta range of the scan to extract
npoints: number of points of the radial scan

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

omrange: integration range in omega 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 two theta positions are returned (default=True)
bounds: flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint: two 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)

Examples

```
>>> 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

omcenter:	om-position at which the 2theta scan should be extracted
ttcenter:	tt-position at which the 2theta scan should be extracted
ttrange:	two theta range of the 2theta scan to extract
npoints:	number of points of the 2theta scan

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

omrange:	integration range in omega direction
lam:	wavelength for use in the conversion to angular coordinates

Returns

qxtt,qztt:	reciprocal 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)

Examples

```
>>>
```

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

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 2theta scan should be extracted
qzcenter:	qz-position at which the 2theta scan should be extracted
ttrange:	two theta range of the scan to extract
npoints:	number of points of the radial scan

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

omrange:	integration range in omega 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 two theta positions are returned (default=True)
bounds:	flag to specify if the scan bounds should be returned :(default: False)

Returns

tt,ttint:	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)

Examples

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

xrayutilities.analysis.line_cuts.**getindex** (*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,y:	coordinates of the point of interest (float)
xgrid,ygrid:	grid coordinates in x and y direction (array)

Returns

ix,iy: index of the closest gridpoint (lower left) of the point (x,y)

xrayutilities.analysis.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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

```
>>> 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

gridder: 3d 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

Examples

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

xrayutilities.analysis.line_cuts3d.**getindex3d** (*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)

xrayutilities.analysis.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

Parameters

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

Examples

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])

xrayutilities.analysis.sample_align module

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

xrayutilities.analysis.sample_align.**area_detector_calib** (*angle1*, *angle2*, *ccdimages*, *detaxis*, *r_i*, *plot=True*, *cut_off=0.7*, *start=(0*, *0*, *0*, *0)*, *fix=(False*, *False*, *False*, *False)*, *fig=None*, *wl=None*, *plotlog=False*, *nwindow=50*, *debug=False*)

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

angle2: inner detector arm angle

ccdimages: images of the ccd taken at the angles given above

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

r_i: primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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. By default (0,0,0,0) is used.
- **fix:** fix parameters of start (default: (False,False,False,False))
- **fig:** matplotlib figure used for plotting the error :default: None (creates own figure)
- **wl:** wavelength of the experiment in Angstrom (default: config.WAVELENGTH) value does not really matter here but does affect the scaling of the error
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to specify that you want to see verbose output and saving of images to show if the CEN determination works

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*, *False)*, *fig=None*, *plotlog=False*, *nwindow=50*, *debug=False*)

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. Both images from the primary beam hkl = (0,0,0) and from a symmetric reflection hkl = (h,k,l) need to be given for a successful run.

parameters

- **sampleang:** sample 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
- **angle1:** outer detector arm angle
- **angle2:** inner detector arm angle
- **ccdimages:** images of the ccd taken at the angles given above
- **hkls:** array/list of hkl values for every image
- **experiment:** Experiment class object needed to get the UB matrix for the hkl peak treatment
- **material:** material used as reference crystal
- **detaxis:** detector arm rotation axis :default: ['z+','y-']
- **r_i:** primary beam direction [xyz][+-] default 'x+'

Keyword_arguments:

- **plot:** flag 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: 0.1 = 10%
- **start:** sequence of start values of the fit for parameters, which can not be estimated automatically. these are: tiltazimuth, tilt, detector_rotation, outerangle_offset, sampletilt, sampletiltazimuth, 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))
- **fig:** matplotlib figure used for plotting the error. :default: None (creates own figure)
- **plotlog:** flag to specify if the created error plot should be on log-scale
- **nwindow:** window size for determination of the center of mass position after the center of mass of every full image is determined, the center of mass is determined again using a window of size nwindow in order to reduce the effect of hot pixels.
- **debug:** flag to tell if you want to see debug output of the script (switch this to true only if you can handle it :))

`xrayutilities.analysis.sample_align.`**`fit_bragg_peak`** (*`om`*, *`tt`*, *`psd`*, *`omalign`*, *`ttalign`*, *`exphxrd`*, *`frange=(0.03`*, *`0.03)`*, *`peaktype='Gauss'`*, *`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) or Lorentzian (xrayutilities.math.Lorentz2d)
PLEASE ALWAYS CHECK THE RESULT CAREFULLY!
Parameters

- **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 +/-frangeAA^{-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})
- **peaktype:** can be 'Gauss' or 'Lorentz' to fit either of the two peak shapes
- **plot:** if True (default) function will plot the result of the fit in comparison with the measurement.

Returns

- **Omfit,ttfit,paramss,covariance:** fitted angular values, and the fit parameters (of the Gaussian/Lorentzian) 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)

keyword arguments:

- **r_i:** primary beam direction as vector [xyz][+-]; default: 'y+'
- **detaxis:** detector arm rotation axis [xyz][+-]; default: 'x+'

other options are passed to psd_chdeg function, options include:

plot: flag to specify if a visualization of the fit should be done

usetilt: whether to use model considering a detector tilt, i.e. 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/pixelwidth*pi/180 ~= 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*, *omega0=None*, *plot=True*)

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

phi: azimuths 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.

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.

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

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'*, *mtiltlabel='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*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, i.e. deviation angle of the pixel direction from orthogonal to the primary beam :(default: True)

datap: plot format of data points

modelline: plot format of modelline

modeltilt: plot format of modeltilt

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/pixelwidth*pi/180 = channel/degree for large detector distance with the sample detector disctance 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

Examples

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

Module contents

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.

xrayutilities.io package

Submodules

xrayutilities.io.cbf module

class xrayutilities.io.cbf.**CBFDirectory** (*datapath*, *ext='cbf'*, ***keyargs*)
Bases: **object**
Parses a directory for CBF files, which can be stored to a HDF5 file for further usage

Save2HDF5 (*h5f*, *group=''*, *comp=True*)
Saves the data stored in the CBF 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.
Parameters

h5f: a HDF5 file object or name

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.cbf.**CBFFile** (*fname*, *nxkey='X-Binary-Size-Fastest-Dimension'*, *nykey='X-Binary-Size-Second-Dimension'*, *dtkey='DataType'*, *path=None*)
Bases: **object**

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

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

xrayutilities.io.cbf.**makeNaturalName** (*name*)

xrayutilities.io.desy_tty08 module

class for reading data + header information from tty08 data files

tty08 is a system used at beamline P08 at Hasylab Hamburg and creates simple ASCII files to save the data. Information is easily read from the multicolumn data file. the functions below enable also to parse the information of the header

xrayutilities.io.desy_tty08.**gettty08_scan** (*scanname*, *scannumbers*, **args*, ***keyargs*)
function to obtain the angular cooridinates as well as intensity values saved in TTY08 datafiles. Especially usefull for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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)

**keyargs: keyword arguments are passed on to tty08File
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']).

Examples

```
>>> [om,tt],MAP = xu.io.gettty08_scan('text%05d.dat',36,'omega','gamma')
```

class xrayutilities.io.desy_tty08.**tty08File** (*filename*, *path=None*, *mcadir=None*)

Bases: **object**

Represents a tty08 data file. The file is read during the Constructor call. This class should work for data stored at beamline P08 using the tty08 acquisition system.

Required constructor arguments:

filename: a string with the name of the tty08-file

Optional keyword arguments:

mcadir: directory name of MCA files

Read ()

Read the data from the file

ReadMCA ()

xrayutilities.io.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 (*h5f*, *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.

Parameters

h5f: a HDF5 file object or name

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*, *keep_open=False*)

Bases: **object**

Parse ()

Parse file to find the number of entries and read the respective header information

ReadData (*nimg=0*)

Read the CCD data of the specified image and return the data this function is called automatically when the 'data' property is accessed, but can also be called manually when only a certain image from the file is needed.

Parameters

nimg: number of the image which should be read (starts with 0)

Save2HDF5 (*h5f*, *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.
Parameters

h5f: a HDF5 file object or name

optional keyword arguments:

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

data

xrayutilities.io.edf.**makeNaturalName** (*name*)

xrayutilities.io.fastscan module

modules to help with the analysis of FastScan data acquired at the ESRF. FastScan data are X-ray data (various detectors possible) acquired during scanning the sample in real space with a Piezo Scanner. The same functions might be used to analze traditional SPEC mesh scans.

The module provides three core classes:

* FastScan * FastScanCCD * FastScanSeries

where the first two are able to parse single mesh/FastScans when one is interested in data of a single channel detector or are detector and the last one is able to parse full series of such mesh scans with either type of detector

see examples/xrayutilities_kmap_ESRF.py for an example script

class xrayutilities.io.fastscan.**FastScan** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **object**
class to help parsing and treating fast scan data. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source.

grid2D (*nx*, *ny*, ***kwargs*)
function to grid the counter data and return the gridded X,Y and Intensity values.
Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))
gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

motorposition (*motorname*)
read the position of motor with name given by motorname from the data file. In case the motor is included in the data columns the returned object is an array with all the values from the file (although retrace clean is respected if already performed). In the case the motor is not moved during the scan only one value is returned.
Parameters

motorname: name of the motor for which the position is wanted

Returns

val: motor position(s) of motor with name motorname during the scan

parse ()
parse the specfile for the scan number specified in the constructor and store the needed informations in the object properties

retrace_clean ()
function to clean the data of the scan from retrace artifacts created by the zig-zag scanning motion of the piezo actuators the function cleans the xvalues, yvalues and data attribute of the FastScan object.

class xrayutilities.io.fastscan.**FastScanCCD** (*filename*, *scannr*, *xmotor='adcX'*, *ymotor='adcY'*, *path=''*)
Bases: **xrayutilities.io.fastscan.FastScan**
class to help parsing and treating fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed

getccdFileTemplate (*specscan*, *datadir=None*, *keepdir=0*, *numfmt='%04d'*)
function to extract the CCD file template string from the comment in the SPEC-file scan-header
Parameters

specscan: spec-scan object from which header the CCD directory should be extracted
datadir: the CCD filenames are usually parsed from the scan object. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.
keepdir: number of directories which should be taken from the specscan. (default: 0)
numfmt: format string for the CCD file number (optional)

Returns

fmtstr: format string for the CCD file name using one number to build the real file name

gridCCD (*nx, ny, ccdnr, roi=None, datadir=None, keepdir=0, nav=[1, 1], gridrange=None, filterfunc=None, imgoffset=0*)
function to grid the internal data and ccd files and return the gridded X,Y and DATA values. DATA represents a 4D with first two dimensions representing X,Y and the remaining two dimensions representing detector channels
Parameters

nx,ny: number of bins in x,y direction
ccdnr: array with ccd file numbers of length length(FastScanCCD.data) OR a string with the data column name for the file ccd-numbers

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

nav: number of detector pixel which will be averaged together (reduces the date size)

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

Returns

X,Y,DATA: regular x,y-grid as well as 4-dimensional data object

class xrayutilities.io.fastscan.**FastScanSeries** (*filenames*, *scannrs*, *nx*, *ny*, **args*, ***kwargs*)

Bases: **object**

class to help parsing and treating a series of fast scan data including CCD frames. FastScan is the aquisition of X-ray data while scanning the sample with piezo stages in real space. It's is available at several beamlines at the ESRF synchrotron light-source. During such fast scan at every grid point CCD frames are recorded and need to be analyzed.

For the series of FastScans we assume that they are measured at different goniometer angles and therefore transform the data to reciprocal space.

align (*deltax*, *deltay*)

Since a sample drift or shift due to rotation often occurs between different FastScans it should be corrected before combining them. Since determining such a shift is not straight-forward in general the user needs to supply the routine with the shifts in order correct the x,y-values for the different FastScans. Such a routine could for example use the integrated CCD intensities and determine the shift using a cross-convolution.

Parameters

deltax: list of shifts in x-direction for every FastScan in the data structure

deltay: same for the y-direction

getCCDFrames (*posx*, *posy*, *typ='real'*)

function to determine the list of ccd-frame numbers for a specific real space position. The real space position must be within the data limits of the FastScanSeries otherwise an ValueError is thrown

Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

Optional:

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

Returns

[[motorpos1, ccdnrs1], [motorpos2, ccdnrs2], ...] where motorposN is

from the N-ths FastScan in the series and ccdnrsN is the list of according CCD-frames

grid2Dall (*nx*, *ny*, ***kwargs*)

function to grid the counter data and return the gridded X,Y and Intensity values from all the FastScanSeries.
Parameters

nx,ny: number of bins in x,y direction

optional keyword arguments:

counter: name of the counter to use for gridding (default: 'mpx4int' (ID01))

gridrange: range for the gridder: format: ((xmin,xmax),(ymin,ymax))

Returns

Gridder2D object with X,Y,data on regular x,y-grid

gridRSM (*posx, posy, qnx, qny, qnz, qconv, roi=None, nav=[1, 1], typ='real', filterfunc=None, **kwargs*)

function to calculate the reciprocal space map at a certain x,y-position from a series of FastScan measurements it is necessary to specify the number of grid-oints for the reciprocal space map and the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.
Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qnx: number of points in the Qx direction of the gridded reciprocal space map

qny: same for y direction

qnz: same for z directino

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

Returns
Gridder3D object with gridded reciprocal space map

rawRSM (*posx, posy, qconv, roi=None, nav=[1, 1], typ='real', datadir=None, keepdir=0, filterfunc=None, **kwargs*)

function to return the reciprocal space map data at a certain x,y-position from a series of FastScan measurements. It necessary to give the QConversion-object to be used for the reciprocal space conversion. The QConversion-object is expected to have the 'area' conversion routines configured properly.
Parameters

posx: real space x-position or index in x direction

posy: real space y-position or index in y direction

qconv: QConversion-object to be used for the conversion of the CCD-data to reciprocal space

Optional:

roi: region of interest on the 2D detector. should be a list of lower and upper bounds of detector channels for the two pixel directions (default: None)

nav: number of detector pixel which will be averaged together (reduces the date size)

typ: type of coordinates. specifies if the position is specified as real space coordinate or as index. valid values are 'real' and 'index'. (default: 'real')

filterfunc: function applied to the CCD-frames before any processing. this function should take a single argument which is the ccddata which need to be returned with the same shape! e.g. remove hot pixels, flat/darkfield correction

UB: sample orientation matrix

datadir: the CCD filenames are usually parsed from the SPEC file. With this option the directory used for the data can be overwritten. Specify the datadir as simple string. Alternatively the innermost directory structure can be automatically taken from the specfile. If this is needed specify the number of directories which should be kept using the keepdir option.

keepdir: number of directories which should be taken from the SPEC file. (default: 0)

Returns

Qx,qy,qz,ccddata,valuelist: raw data of the reciprocal space map and valuelist containing the ccdframe numbers and corresponding motor positions

read_motors ()
read motor values from the series of fast scans

retrace_clean ()
perform retrace clean for every FastScan in the series

xrayutilities.io.helper module

convenience functions to open files for various data file reader

these functions should be used in new parsers since they transparently allow to open gzipped and bzipped files

class xrayutilities.io.helper.**xu_h5open** (*f*, *mode='r'*)
Bases: **object**
helper object to decide if a HDF5 file has to be opened/closed when using with a 'with' statement.

xrayutilities.io.helper.**xu_open** (*filename*, *mode='rb'*)
function to open a file no matter if zipped or not. Files with extension '.gz' or '.bz2' are assumed to be compressed and transparently opened to read like usual files.
Parameters

filename: filename of the file to open (full including path)

mode: mode in which the file should be opened

Returns

file handle of the opened file

If the file does not exist an IOError is raised by the open routine, which is not caught within the function

xrayutilities.io.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 with

1. RoperScientific files with 4096x4096 pixels created at Hasylab Hamburg, which save an 16bit integer per point.
2. Perkin Elmer images created at Hasylab Hamburg with 2048x2048 pixels.

readImage (*filename*, *path=None*)
read image file and correct for dark- and flatfield in case the necessary data are available.
returned data = ((image data)-(darkfield))/flatfield*average(flatfield)
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed. supported extensions: .tif, .bin and .bin.xz

class xrayutilities.io.imagereader.**PerkinElmer** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse PerkinElmer CCD frames (*.tif) 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.**Pilatus100K** (***keyargs*)
Bases: **xrayutilities.io.imagereader.ImageReader**
parse Dectris Pilatus 100k frames (*.tiff) to numpy arrays Ignore the header since it seems to contain no useful data

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.

class xrayutilities.io.imagereader.**TIFFRead** (*filename*, *path=None*)
Bases: **xrayutilities.io.imagereader.ImageReader**
class to Parse a TIFF file including extraction of information from the file header in order to determine the image size and data type
The data stored in the image are available in the 'data' property.

xrayutilities.io.imagereader.**get_tiff** (*filename*, *path=None*)
read tiff image file and return the data
Parameters

filename: filename of the image to be read. so far only single filenames are supported. The data might be compressed.

xrayutilities.io.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*, *path=''*)
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*, *namespace=''*)
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.XRDMLFile class is used. The function can be used for parsing maps measured with the PIXCel 1D detector (and in limited way also for data acquired with a point detector -> see getxrdml_scan instead).
Parameters

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 usefull!

Returns

om,tt,psd: as flattened numpy arrays

Examples

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

xrayutilities.io.panalytical_xml.**getxrdml_scan** (*filetemplate*, **motors*, ***kwargs*)
parses multiple XRDML file and concatenates the results for parsing the xrayutilities.io.XRDMLFile class is used. The function can be used for parsing arbitrary scans and will return the the motor values of the scan motor and additionally the positions of the motors given by in the "*motors" argument
Parameters

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

***motors: motor names to return: e.g.: 'Omega','2Theta',...**

one can also use abbreviations 'Omega' = 'om' = 'o' '2Theta' = 'tt' = 't' 'Chi' = 'c' 'Phi' = 'p'

****kwargs:**

scannrs: int or list of scan numbers
path: common path to the filenames

Returns

scanmot,mot1,mot2,...,detectorint: as flattened numpy arrays

Examples

```
>>> scanmot,om,tt,inte = xrayutilities.io.getxrdml_scan(
        "samplename_1.xrdml", 'om', 'tt', path="./data")
```

xrayutilities.io.pdcif module

class xrayutilities.io.pdcif.**pdCIF** (*filename*, *datacolumn=None*)
Bases: **object**
the class implements a primitive parser for pdCIF-like files. It reads every entry and collects the information in the header attribute. The first loop containing one of the intensity fields is assumed to be the data the user is interested in and is transfered to the data array which is stored as numpy record array the columns can be accessed by name

intensity fields:

_pd_meas_counts_total, _pd_meas_intensity_total, _pd_proc_intensity_total, _pd_proc_intensity_net, _pd_calc_intensity_total, _pd_calc_intensity_net

alternatively the data column name can be given as argument to the constructor

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

class xrayutilities.io.pdcif.**pdESG** (*filename*, *datacolumn=None*)
Bases: **xrayutilities.io.pdcif.pdCIF**
class for parsing multiple pdCIF loops in one file. This includes especially *.esg files which are supposed to consist of multiple loops of pdCIF data with equal length.
Upon parsing the class tries to combine the data of these different scans into a single data matrix -> same shape of subscan data is assumed

Parse ()
parser of the pdCIF file. the method reads the data from the file and fills the data and header attributes with content

xrayutilities.io.pdcif.**remove_comments** (*line*, *sep='#'*)

xrayutilities.io.rigaku_ras module

class for reading data + header information from Rigaku RAS (3-column ASCII) files

Such datafiles are generated by the Smartlab Guidance software from Rigaku.

class xrayutilities.io.rigaku_ras.**RASFile** (*filename*, *path=None*)
Bases: **object**
Represents a RAS data file. The file is read during the constructor call
Required constructor arguments:

filename: a string with the name of the ras-file

keyword argument (optional):

path: path to the data file

Read ()
Read the data from the file

class xrayutilities.io.rigaku_ras.**RASScan** (*filename*, *pos*)
Bases: **object**
Represents a single Scan portion of a RAS data file. The scan is parsed during the constructor call
Required constructor arguments:

filename: file name of the data file
pos: seek position of the RAS_HEADER_START line

xrayutilities.io.rigaku_ras.**getras_scan** (*scanname*, *scannumbers*, **args*, ***kwargs*)
function to obtain the angular cooridinates as well as intensity values saved in RAS datafiles. Especially useful for reciprocal space map measurements, and to combine date from several scans
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

scanname: name of the scans, for multiple scans this needs to be a template string
scannumbers: 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: keyword arguments forwarded to RASFile function
Returns

rasdata

or

[ang1,ang2,...],rasdata:

angular positions are extracted from the respective scan header together with all the data values as stored in the data file (includes the intensities e.g. rasdata['int']).

Examples

```
>>> [om,tt],MAP = xu.io.getras_scan('text%05d.ras',36,'Omega','TwoTheta')
```

xrayutilities.io.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

xrayutilities.io.seifert module

a set of routines to convert Seifert ASCII files to HDF5 in fact there exist two posibilities 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**

helper class to represent a Seifert (NJA) scan file header

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

Bases: **object**

Class to parse a Seifert (NJA) multiscan file

parse ()

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

Bases: **object**

Class to parse a single Seifert (NJA) scan file

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.
Parameters

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: can be either "map" (reciprocal space map measured with a regular Seifert job (default)) or "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

Examples

```
>>> 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 preceeding _.

xrayutilities.io.spec module

a 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`**

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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

comp: activate 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**
class to parse a SPEC log file to find the command history

Parse ()

class xrayutilities.io.spec.**SPECScan** (*name*, *scannr*, *command*, *date*, *time*, *itime*, *colnames*, *hoffset*, *doffset*, *fname*, *imopnames*, *imopvalues*, *scan_status*)
Bases: **object**
Represents a single SPEC scan. This class is usually not called by the user directly but used via the SPECFile class.

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=''*, *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 ususally 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:

h5f: a HDF5 file object or its filename

optional keyword arguments:

group: name or group object of the HDF5 group where to store the data
title: a string with the title for the data, defaults to the name of scan if empty
optattrs: a dictionary with optional attributes to store for the data
comp: activate 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 aguments:

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*, ***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:**

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 cooridinates as well as intensity values saved in an HDF5 file, which was created from a spec file by the Save2HDF5 method. Especially useful 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 h5py 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 ommited the first child node of h5f.root will be used

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

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']).

Examples

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

xrayutilities.io.spec.**getspec_scan** (*specf*, *scans*, **args*, ***kwargs*)

function to obtain the angular cooridinates as well as intensity values saved in a SPECFile. Especially useful to combine the data from multiple scans.
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

specf: SPECFile object

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

args: names of the motors and counters (strings)

keyword arguments:

rettype: how to return motor positions. by default a list of arrays is returned. when rettype == 'numpy' a record array will be returned.

Returns

[ang1,ang2,...]:

coordinates and counters from the SPEC file

Examples

```
>>> [om, tt, cnt2] = xu.io.getspec_scan(s, 36, 'omega', 'gamma',
                                        'Counter2')
```

xrayutilities.io.spec.**makeNaturalName** (*name*)

xrayutilities.io.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='/'*, *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

name: name of the group where to store the data

optional keyword arguments:

group: root group where to store the data

mcaname: Name of the MCA in the HDF5 file

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**

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

h5f: file object of a HDF5 file opened using h5py

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

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

omname: name of the omega motor (or its equivalent)

ttname: name of the two theta motor (or its equivalent)

****kwargs (optional):**

mca: name 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']).

Module contents

xrayutilities.materials package

Submodules

xrayutilities.materials.atom module

module containing the Atom class which handles the database access for atomic scattering factors and the atomic mass.

class xrayutilities.materials.atom.**Atom** (*name*, *num*)

Bases: **object**

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

function to calculate the atomic structure factor F

Parameters

q: momentum transfer

en: 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'*)

weight

xrayutilities.materials.cif module

class xrayutilities.materials.cif.**CIFFile** (*filename*, *digits=3*)

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.

xrayutilities.materials.database module

module to handle the access to the optical parameters database

class xrayutilities.materials.database.**DataBase** (*fname*)
Bases: **object**

Close ()
Close an opend 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*, *dset='default'*)
Obtain the f0 scattering factor component for a particular momentum transfer q.

required input argument:

q: single float value or numpy array
dset: specifies which dataset (different oxidation states) should be used

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*, *subset='default'*)
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
subset: specifies under which name the f0 values should be saved

SetF1F2 (*en*, *f1*, *f2*)
Set f1, f2 values for the active material.

required input arguments:

en: list or numpy array with energy in (eV)
f1: list or numpy array with f1 values
f2: list 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:

name: string with the name of the material

SetWeight (*weight*)
Save weight of the element as float

required input argument:

weight: atomic standard weight of the element (float)

xrayutilities.materials.database.**add_f0_from_intertab** (*db*, *itf*)
Read f0 data from International Tables of Crystallography and add it to the database.

xrayutilities.materials.database.**add_f0_from_xop** (*db*, *xop*)
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*, *hf*)
Read f1 and f2 data from Henke database and add it to the database.

xrayutilities.materials.database.**add_f1f2_from_kissel** (*db*, *kf*)
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. The mass of the natural isotope mixture is taken from the NIST data!

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

xrayutilities.materials.elements module

xrayutilities.materials.lattice module

module handling crystal lattice structures. A Lattice consists of unit cell parameters and a LatticeBase. It offers methods to calculate the reciprocal space position of Bragg peaks and their structure factor.

xrayutilities.materials.lattice.**AlGaAsLattice** (*aal*, *aga*, *aas*, *a*, *x*)

xrayutilities.materials.lattice.**BCCLattice** (*aa*, *a*)

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

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

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

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

xrayutilities.materials.lattice.**CubicLattice** (*a*, *base=None*)

Returns a Lattice object representing a cubic lattice.
Parameters

a: lattice parameter
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

xrayutilities.materials.lattice.**DiamondLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCLattice** (*aa*, *a*)

xrayutilities.materials.lattice.**FCCSharedLattice** (*aa*, *ab*, *occa*, *occb*, *a*)

xrayutilities.materials.lattice.**GeTeRhombohedral** (*aa*, *ab*, *a*, *ang*, *x=0.237*)

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*)

xrayutilities.materials.lattice.**HexagonalLattice** (*a*, *c*, *base=None*)
Returns a Lattice object representing a hexagonal lattice.
Parameters

a: lattice parameter a
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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 and unit cell defined by three vectors.

ApplyStrain (*eps*)
Applies a certain strain on a lattice. The result is a change in the base vectors. The full strain matrix (3x3) needs to be given. .. note:: Note: NO elastic response of the material will be considered!

requiered input arguments:

eps: a 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 (angstrom^3)

a

a1

a2

a3

alpha

b

beta

c

gamma

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

Parameters

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*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.**MagnetiteLattice** (*aa*, *ab*, *ac*, *a*, *x=0.255*)

xrayutilities.materials.lattice.**MonoclinicLattice** (*a*, *b*, *c*, *beta*, *base=None*)

Returns a Lattice object representing a hexagonal lattice.

Parameters

a: lattice parameter a

b: lattice parameter b

c: lattice parameter c

beta: monoclinic unit cell angle beta (deg)

base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

xrayutilities.materials.lattice.**NiAsLattice** (*aa*, *ab*, *a*, *c*, *biso=0.0*)

xrayutilities.materials.lattice.**OrthorhombicLattice** (*a*, *b*, *c*, *base=None*)

Returns a Lattice object representing a tetragonal lattice.

Parameters

a: lattice parameter a

b: lattice parameter b

c: lattice parameter c

base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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*)
creates the primitive unit cell of a RockSalt structure. For the more commonly used cubic reprentation see RockSalt_Cubic_Lattice

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

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

xrayutilities.materials.lattice.**SiGeLattice** (*asi*, *age*, *a*, *xge*)

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

xrayutilities.materials.lattice.**TetragonalLattice** (*a*, *c*, *base=None*)
Returns a Lattice object representing a tetragonal lattice.
Parameters

a: lattice parameter a
c: lattice parameter c
base: instance of LatticeBase, representing the internal structure of the unit cell

Returns

an instance of Lattice class

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

xrayutilities.materials.lattice.**TriclinicLattice** (*a*, *b*, *c*, *alpha*, *beta*, *gamma*, *base=None*)

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*)

xrayutilities.materials.material module

Classes decribing materials. Materials are devided with respect to their crystalline state in either Amorphous or Crystal types. While for most materials their crystalline state is defined few materials are also included as amorphous which can be useful for calculation of their optical properties.

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

RelaxationTriangle (*hkl*, *sub*, *exp*)
function which returns the relaxation trianlge for a Alloy of given composition. Reciprocal space coordinates are calculated using the user-supplied experimental class
Parameters

hkl: Miller Indices
sub: substrate material or lattice constant (Instance of Crystal 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

class xrayutilities.materials.material.**Amorphous** (*name*, *density*, *atoms=None*, *cij=None*)
Bases: **xrayutilities.materials.material.Material**
amorphous materials are described by this class

beta (*en='config'*)
function to calculate the imaginary part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

delta (*en='config'*)
function to calculate the real part of the deviation of the refractive index from 1 (n=1-delta+i*beta)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

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.**Crystal** (*name*, *lat*, *cij=None*, *thetaDebye=None*)
Bases: **xrayutilities.materials.material.Material**
Crystalline materials are described by this class

ApplyStrain (*strain*)
Applies a certain strain on the lattice of the material. The result is a change in the base vectors of the real space as well as reciprocal space lattice. The full strain matrix (3x3) needs to be given. Note: NO elastic response of the material will be considered!

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.
Parameters

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
Parameters

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
Parameters

q0: vectorial momentum transfer (vectors as list,tuple or numpy array are valid)
en: list, tuple or array of energy values in eV
temp: temperature 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
Parameters

q: vectorial 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)])
en0: energy value in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature 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)
Parameters

en: x-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 + chi_r0/2 + i*chi_i0/2 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
Parameters

q: momentum transfer in (1/A)
en: xray energy in eV, if omitted the value from the xrayutilities configuration is used
temp: temperature used for Debye-Waller-factor calculation
polarization: either 'S' (default) sigma or 'P' pi polarization

Returns

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

dTheta (*Q*, *en='config'*)
function to calculate the refractive peak shift
Parameters

Q: momentum transfer (1/A)
en: x-ray energy (eV), if omitted the value from the xrayutilities configuration is used

Returns

deltaTheta: peak 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)
Parameters

en: x-ray energy eV, if omitted the value from the xrayutilities configuration is used

Returns

delta (float)

density
calculates the mass density of an material from the mass of the atoms in the unit cell.
Returns
mass density in kg/m^3

distances ()
function to obtain distances of atoms in the crystal up to the unit cell size (largest value of a,b,c is the cut-off)
returns a list of tuples with distance d and number of occurence n [(d1,n1),(d2,n2),...]

Note

Note: if the base of the material is empty the list will be empty

environment (pos*, ***kwargs*)**
Returns a list of neighboring atoms for a given position within the the unit cell.
Parameters

pos: list or numpy array with the fractional coordinated in the unit cell

keyword arguments:

maxdist: maximum distance wanted in the list of neighbors :(default: 7)

Returns

list of tuples with (distance,atomType,multiplicity) giving distance (sorted) and type of neighboring atoms together with the amount of atoms at the given distance

classmethod **fromCIF** (*ciffilename*)

Create a Crystal from a CIF file. Name and

Parameters

ciffilename: filename of the CIF file

Returns

Crystal instance

planeDistance (hkl*)**

determines the lattice plane spacing for the planes specified by (hkl)

Parameters

h,k,l: Miller indices of the lattice planes given either as list,tuple or seperate arguments

Returns

d: the lattice plane spacing as float

Examples

```
>>> xu.materials.Si.planeDistance(0,0,4)
1.3577600000000001
```

or

```
>>> xu.materials.Si.planeDistance((1,1,1))
3.1356124059796255
```

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

Parameters

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 symetric peak. As an additional input the substrates lattice parameter and the degree of relaxation must be given

Parameters

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

Parameters

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'*, *base=None*)

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

Parameters

a,b,c: unit cell extenstions (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

base: instance of LatticeBase

returns a Crystal 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

Parameters

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*, *cij=None*)

Bases: **object**

base class for all Materials. common properties of amorphous and crystalline materials are described by this class from which Amorphous and Crystal are derived from.

beta (*en='config'*)

chi0 (*en='config'*)

calculates the complex chi_0 values often needed in simulations. They are closely related to delta and beta (n = 1 + chi_r0/2 + i*chi_i0/2 vs. n = 1 - delta + i*beta)

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

calculate critical angle for total external reflection

Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

deg: return angle in degree if True otherwise radians (default:True)

Returns

Angle of total external reflection

delta (*en='config'*)

density

idx_refraction (*en='config'*)
function to calculate the complex index of refraction of a material in the x-ray range
Parameters

en: energy of the x-rays, if omitted the value from the xrayutilities configuration is used

Returns

n (complex)

lam

mu

nu

xrayutilities.materials.material.**PseudomorphicMaterial** (*sub*, *layer*, *relaxation=0*, *trans=None*)
This function returns a material whos lattice is pseudomorphic on a particular substrate material. The two materials must have similar unit cell definitions for the algorithm to work correctly, i.e. it does not work for combiniations of materials with different lattice symmetry.
Parameters

sub: substrate material
layer: bulk material of the layer
relaxation: degree of relaxation 0: pseudomorphic, 1: relaxed :(default: 0)
trans: Transformation which transforms lattice directions into a surface orientated coordinate frame (x,y inplane, z out of plane). If None a (001) surface geometry of a cubic material is assumed.

Returns
An instance of Crystal holding the new pseudomorphically strained material.

xrayutilities.materials.material.**WZTensorFromCub** (*c11ZB*, *c12ZB*, *c44ZB*)
Determines the hexagonal elastic tensor from the values of the cubic elastic tensor under the assumptions presented in Phys. Rev. B 6, 4546 (1972), which are valid for the WZ <-> ZB polymorphs.
Parameters

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

Returns

6x6 matrix with elastic constants
Implementation according to a patch submitted by Julian Stangl

xrayutilities.materials.material.**index_map_ij2ijkl** (*ij*)

xrayutilities.materials.material.**index_map_ijkl2ij** (*i*, *j*)

xrayutilities.materials.predefined_materials module

class xrayutilities.materials.predefined_materials.**AlGaAs** (*x*)
Bases: **xrayutilities.materials.material.CubicAlloy**

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

Module contents

xrayutilities.math package

Submodules

xrayutilities.math.algebra module

module providing analytic algebraic functions not implemented in scipy or any other dependency of xrayutilities. In particular the analytic solution of a quartic equation which is needed for the solution of the dynamic scattering equations.

`xrayutilities.math.algebra.`**`solve_quartic`** (*a4*, *a3*, *a2*, *a1*, *a0*)
analytic solution [1] of the general quartic equation. The solved equation takes the form:
a4*z**4 + a3*z**3 + a2*z**2 + a1*z + a0
Returns

tuple of the four (complex) solutions of aboves equation.
[1] http://mathworld.wolfram.com/QuarticEquation.html

xrayutilities.math.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,y:	data coordinates (do NOT need to be regularly spaced)
data:	data set used for fitting (e.g. intensity at the data coords)
start:	set of starting parameters for the fit used as first parameter of function fit_function
drange:	limits 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_function:	function 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=300*)
Gauss fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting
Parameters

xdata:	xcoordinates of the data to be fitted
ydata:	ycoordinates of the data which should be fit

keyword parameters:

iparams:	initial paramters for the fit, determined automatically if not given
maxit:	maximal 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

`xrayutilities.math.fit.`**`linregress`** (*x*, *y*)
fast linregress to avoid usage of scipy.stats which is slow!
Parameters

x,y:	data coordinates and values

Returns

p, rsq: parameters of the linear fit (slope, offest) and the R^2 value
Examples

```
>>> (k, d), R2 = xu.math.linregress(x, y)
```

xrayutilities.math.fit.**multGaussFit** (**args*, ***kwargs*)
convenience function to keep API stable see multPeakFit for documentation

xrayutilities.math.fit.**multGaussPlot** (**args*, ***kwargs*)
convenience function to keep API stable see multPeakPlot for documentation

xrayutilities.math.fit.**multPeakFit** (*x*, *data*, *peakpos*, *peakwidth*, *dranges=None*, *peaktype='Gaussian'*)
function to fit multiple Gaussian/Lorentzian peaks with linear background to a set of data
Parameters

x:	x-coordinate of the data
data:	data array with same length as x
peakpos:	initial parameters for the peak positions
peakwidth:	initial values for the peak width
dranges:	list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as peakpos
peaktype:	type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'

Returns

pos,sigma,amp,background

Pos:	list of peak positions derived by the fit
Sigma:	list of peak width derived by the fit
Amp:	list of amplitudes of the peaks derived by the fit
Background:	array of background values at positions x

xrayutilities.math.fit.**multPeakPlot** (*x*, *fpos*, *fwidth*, *famp*, *background*, *dranges=None*, *peaktype='Gaussian'*, *fig='xu_plot'*, *fact=1.0*)
function to plot multiple Gaussian/Lorentz peaks with background values given by an array
Parameters

x:	x-coordinate of the data
fpos:	list of positions of the peaks
fwidth:	list of width of the peaks
famp:	list of amplitudes of the peaks
background:	array with background values
dranges:	list of tuples with (min,max) value of the data ranges to use. does not need to have the same number of entries as fpos
peaktype:	type of peaks to be used: can be either 'Gaussian' or 'Lorentzian'
fig:	matplotlib figure number or name
fact:	factor to use as multiplicator in the plot

xrayutilities.math.fit.**peak_fit** (*xdata*, *ydata*, *iparams=[]*, *peaktype='Gauss'*, *maxit=300*, *background='constant'*, *plot=False*, *func_out=False*, *debug=False*)
fit function using odr-pack wrapper in scipy similar to :https://github.com/tiagopereira/python_tips/wiki/Scipy%3A-curve-fitting for Gauss, Lorentz or Pseudovoigt-functions
Parameters

xdata:	xcoordinates of the data to be fitted
ydata:	ycoordinates of the data which should be fit

keyword parameters:

iparams:	initial paramters for the fit, determined automatically if not specified
peaktype:	type of peak to fit: 'Gauss', 'Lorentz', 'PseudoVoigt', 'PseudoVoigtAsym'

maxit: maximal iteration number of the fit

background: type of background, either 'constant' or 'linear'

plot: flag to ask for a plot to visually judge the fit. If plot is a string it will be used as figure name, which makes reusing the figures easier.

func_out: returns the fitted function, which takes the independent variables as only argument (f(x))

Returns

params,sd_params,itlim[,fitfunc]

the parameters as defined in function Gauss1d/Lorentz1d/PseudoVoigt1d/ PseudoVoigt1dasym(x, *param). In the case of linear background one more parameter is included! For every parameter the corresponding errors of the fit 'sd_params' are returned. A boolean flag 'itlim', which is False in the case of a successful fit is added by default. Further the function used in the fit can be returned (see func_out).

xrayutilities.math.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
Examples
Calling with a list of parameters needs a call looking as shown below (note the '*') or explicit listing of the parameters: >>> Gauss1d(x,*p) >>> Gauss1d(numpy.linspace(0,10,100), 5, 1, 1e3, 0)

`xrayutilities.math.functions.`**`Gauss1dArea`** (**p*)

function to calculate the area of a Gauss function with neglected background
Parameters

p: list of parameters of the Gauss-function [XCEN,SIGMA,AMP,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

`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.`**`Gauss2dArea`** (**p*)
function to calculate the area of a 2D Gauss function with neglected background
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,SIGMAX,SIGMAY,AMP,ANGLE,BACKGROUND]

Returns
the area of the Gaussian described by the parameters p

`xrayutilities.math.functions.`**`Gauss3d`** (*x*, *y*, *z*, **p*)
function to calculate a general three dimensional Gaussian
Parameters

p: list of parameters of the Gauss-function [XCEN,YCEN,ZCEN,SIGMAX,SIGMAY,SIGMAZ,AMP,BACKGROUND] SIGMA = FWHM / (2*sqrt(2*log(2)))

x,y,z: coordinate(s) where the function should be evaluated

Returns
the value of the Gaussian described by the parameters p at positions (x,y,z)

`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: 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.`**`Lorentz1dArea`** (**p*)
function to calculate the area of a Lorentz function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND]

Returns
the area of the Lorentzian described by the parameters p

`xrayutilities.math.functions.`**`Lorentz1d_der_p`** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect the parameters p
for parameter description see Lorentz1d

`xrayutilities.math.functions.`**`Lorentz1d_der_x`** (*x*, **p*)
function to calculate the derivative of a Gaussian with respect to x
for parameter description see Lorentz1d

`xrayutilities.math.functions.`**`Lorentz2d`** (*x*, *y*, **p*)
function to calculate a general two dimensional Lorentzian
Parameters

p: list 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,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.**NormGauss1d** (*x*, **p*)
function to calculate a normalized one dimensional Gaussian
Parameters

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

x: coordinate(s) where the function should be evaluated

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

xrayutilities.math.functions.**PseudoVoigt1d** (*x*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

xrayutilities.math.functions.**PseudoVoigt1dArea** (**p*)
function to calculate the area of a pseudo Voigt function with neglected background
Parameters

p: list of parameters of the Lorentz-function [XCEN,FWHM,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the area of the PseudoVoigt described by the parameters p

xrayutilities.math.functions.**PseudoVoigt1d_der_p** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect the parameters p
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1d_der_x** (*x*, **p*)
function to calculate the derivative of a PseudoVoigt with respect to x
for parameter description see PseudoVoigt1d

xrayutilities.math.functions.**PseudoVoigt1dasym** (*x*, **p*)
function to calculate an asymmetric pseudo Voigt function as linear combination of asymmetric Gauss and Lorentz peak
Parameters

p: list of parameters of the pseudo Voigt-function [XCEN,FWHMLEFT,FWHMRIGHT,AMP,BACKGROUND,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

x: coordinate(s) where the function should be evaluated

Returns
the value of the PseudoVoigt described by the parameters p at position 'x'

xrayutilities.math.functions.**PseudoVoigt2d** (*x*, *y*, **p*)
function to calculate a pseudo Voigt function as linear combination of a Gauss and Lorentz peak in two dimensions
Parameters

x,y: coordinate(s) where the function should be evaluated

p: list of parameters of the pseudo Voigt-function [XCEN,YCEN,FWHMX,FWHMY,AMP,BACKGROUND,ANGLE,ETA] :ETA: 0 ...1 0 means pure Gauss and 1 means pure Lorentz

Returns
the value of the PseudoVoigt 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

p: list of parameters of the Gauss-function [XCEN1,YCEN1,SIGMAX1,SIGMAY1,AMP1,ANGLE1,XCEN2,YCEN2, SIGMAX2,SIGMAY2,AMP2,ANGLE2,BACKGROUND] 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.`**`heaviside`** (*x*)
Heaviside step function for numpy arrays
Parameters

x: any scalar of ndarray object

Returns

s: Heaviside step function evaluated for all values of x

`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

data: 1d numpy array with experimental data

threshold: threshold factor to identify strange data points

Returns

1d data-array with spikes removed

`xrayutilities.math.functions.`**`multPeak1d`** (*x*, *`*args`*)
function to calculate the sum of multiple peaks in 1D. the peaks can be of different type and a background function (polynom) can also be included.
Parameters

x: coordinate where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'a': asym. PseudoVoigt, 'p': polynom the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss1d, math.Lorentz1d, math.PseudoVoigt1d, math.PseudoVoigt1dasym, and numpy.polyval for details of the different function types.

Returns

value of the sum of functions at position x

`xrayutilities.math.functions.`**`multPeak2d`** (*x*, *y*, *`*args`*)
function to calculate the sum of multiple peaks in 2D. the peaks can be of different type and a background function (polynom) can also be included.
Parameters

x,y: coordinates where the function should be evaluated

args: list of peak/function types and parameters for every function type two arguments need to be given first the type of function as string with possible values 'g': Gaussian, 'l': Lorentzian, 'v': PseudoVoigt, 'c': constant the second type of arguments is the tuple/list of parameters of the respective function. See documentation of math.Gauss2d, math.Lorentz2d, math.PseudoVoigt2d for details of the different function types. The constant accepts a single float which will be added to the data

Returns

value of the sum of functions at position (x,y)

`xrayutilities.math.functions.`**`smooth`** (*x*, *n*)
function to smooth an array of data by averaging N adjacent data points
Parameters

x: 1D data array

n: number of data points to average

Returns

xsmooth: smoothed array with same length as x

xrayutilities.math.misc module

`xrayutilities.math.misc.`**`center_of_mass`** (*pos*, *data*, *background='none'*, *full_output=False*)
function to determine the center of mass of an array
Parameters

pos: position of the data points

data: data values

background: type of background, either 'none', 'constant' or 'linear'

full_output: return background cleaned data and background-parameters

Returns

center of mass position (single float)

`xrayutilities.math.misc.`**`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)
Parameters

pos: position of the data points

data: data values

Returns

fwhm value (single float)

xrayutilities.math.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.

class `xrayutilities.math.transforms.`**`AxisToZ_keepXY`** (*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/y-axis of the new coordinate frame is created to be similar to the old x and y directions. This variant of AxisToZ assumes that the new Z-axis has its main component along the Z-direction

`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*, *rank=1*)

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 size of the transformation matrix.

rank: rank of the supplied object. allowed values are 1, 2, and 4

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 radiants.

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 radiants.

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 radiants.

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

Parameters

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

Examples

```
>>> 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

xrayutilities.math.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)*norm(v2)*cos(alpha*)

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 radiants

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

Module contents

xrayutilities.simpack package

Submodules

xrayutilities.simpack.fit module

xrayutilities.simpack.fit.**fit_xrr** (*reflmod*, *params*, *ai*, *data=None*, *eps=None*, *xmin=-inf*, *xmax=inf*, *plot=False*, *verbose=False*, *elog=True*, *maxfev=500*)
optimize function for a Reflectivity Model using lmfit. The fitting parameters must be specified as instance of lmfits Parameters class.
Parameters

reflmod: preconfigured SpecularReflectivityModel

params: instance of lmfits Parameters class. For every layer the parameters '{}_thickness', '{}_roughness', '{}_density', with '{}' representing the layer name are supported. In addition the setup parameters: - 'I0' primary beam intensity - 'background' background added to the simulation - 'sample_width' size of the sample along the beam - 'beam_width' width of the beam in the same units - 'resolution_width' width of the resolution function in deg - 'shift' experimental shift of the incidence angle array

ai: array of incidence angles for the calculation

data: experimental data which should be fitted

eps: (optional) error bar of the data

xmin: minimum value of ai which should be used. a mask is generated to cut away other data

xmax: maximum value of ai which should be used. a mask is generated to cut away other data

plot: flag to decide wheter an plot should be created showing the fit's progress. If plot is a string it will be used as figure name, which makes reusing the figures easier.

verbose: flag to tell if the variation of the fitting error should be output during the fit.

elog: logarithmic error during the fit

maxfev: maximum number of function evaluations during the leastsq optimization

Returns

res: MinimizerResult object from lmfit, which contains the fitted parameters in res.params (see res.params.pretty_print) or try lmfit.report_fit(res)

xrayutilities.simpack.models module

class xrayutilities.simpack.models.**DynamicalModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.SimpleDynamicalCoplanarModel**
Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a generalized 2-beam theory (4 tiepoints, S and P polarizations)
The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*)
performs the actual diffraction calculation for the specified incidence angles and uses an analytic solution for the quartic dispersion equation
Parameters

alphai: vector of incidence angles (deg)
hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)
geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**KinematicalModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.LayerModel**
Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of one (hkl) Bragg peak, however considers the variation of the structure factor for different 'q'. The surface geometry is specified using the Experiment-object given to the constructor.

init_chi0 ()
calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness does NOT require this!)

simulate (*qz*, *hkl*, *absorption=False*, *refraction=False*)
performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a single Bragg peak.
Parameters

qz: simulation positions along qz
hkl: Miller indices of the Bragg peak whos truncation rod should be calculated
absorption: flag to tell if absorption correction should be used
refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**KinematicalMultiBeamModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.KinematicalModel**
Kinematical diffraction model for specular and off-specular qz-scans. The model calculates the kinematical contribution of several Bragg peaks on the truncation rod and considers the variation of the structure factor. In order to use a analytical description for the kinematic diffraction signal all layer thicknesses are changed to a multiple of the respective lattice parameter along qz. Therefore this description only works for (001) surfaces.

simulate (*qz*, *hkl*, *absorption=False*, *refraction=True*)
performs the actual kinematical diffraction calculation on the Qz positions specified considering the contribution from a full truncation rod
Parameters

qz: simulation positions along qz
hkl: Miller indices of the Bragg peak whos truncation rod should be calculated
absorption: flag to tell if absorption correction should be used
refraction: flag to tell if basic refraction correction should be performed. If refraction is True absorption correction is also included independent of the absorption flag.

Returns

vector of the ratios of the diffracted and primary fluxes

class xrayutilities.simpack.models.**LayerModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.Model**
generic model class from which further thin film models can be derived from

class xrayutilities.simpack.models.**Model** (*experiment*, ***kwargs*)
Bases: **object**
generic model class from which further models can be derived from

convolute_resolution (*x*, *y*)
convolve simulation result with a Gaussian resolution function
Parameters

x: x-values of the simulation, units of x also decide about the unit of the resolution_width parameter

y: y-values of the simulation

Returns

convoluted y-data with same shape as y

scale_simulation (*y*)
scale simulation result with primary beam flux/intensity and add a background.
Parameters

y: y-values of the simulation

Returns

scaled y values

class xrayutilities.simpack.models.**SimpleDynamicalCoplanarModel** (**args*, ***kwargs*)
Bases: **xrayutilities.simpack.models.KinematicalModel**
Dynamical diffraction model for specular and off-specular qz-scans. Calculation of the flux of reflected and diffracted waves for general asymmetric coplanar diffraction from an arbitrary pseudomorphic multilayer is performed by a simplified 2-beam theory (2 tiepoints, S and P polarizations)
No restrictions are made for the surface orientation.
The first layer in the model is always assumed to be the semiinfinite substrate indepentent of its given thickness

Note

Note: This model should not be used in real life scenarios since the made approximations severely fail for distances far from the reference position.

get_polarizations ()
return list of polarizations which should be calculated

join_polarizations (*Is*, *Ip*)
method to calculate the total diffracted intensity from the intensities of S and P-polarization.

set_hkl (hkl*)**
To speed up future calculations of the same Bragg peak optical parameters can be pre-calculated using this function.
Parameters

hkl: Miller indices of the Bragg peak for the calculation

simulate (*alphai*, *hkl=None*, *geometry='hi_lo'*, *idxref=1*)
performs the actual diffraction calculation for the specified incidence angles.
Parameters

alphai: vector of incidence angles (deg)

hkl: Miller indices of the diffraction vector (preferable use set_hkl method to speed up repeated calculations of the same peak!)

geometry: 'hi_lo' for grazing exit (default) and 'lo_hi' for grazing incidence

idxref: index of the reference layer. In order to get accurate peak position of the film peak you want this to be the index of the film peak (default: 1). For the substrate use 0.

Returns

vector of intensities of the diffracted signal

class xrayutilities.simpack.models.**SpecularReflectivityModel** (**args*, ***kwargs*)

Bases: **xrayutilities.simpack.models.LayerModel**

model for specular reflectivity calculations

densityprofile (*nz*, *plot=False*)

calculates the electron density of the layerstack from the thickness and roughness of the individual layers

Parameters

nz: number of values on which the profile should be calculated

plot: flag to tell if a plot of the profile should be created

Returns

z, eprof: coordinates and electron profile. z = 0 corresponds to the

surface

init_cd ()

calculates the needed optical parameters for the simulation. If any of the materials/layers is changing its properties this function needs to be called again before another correct simulation is made. (Changes of thickness and roughness do NOT require this!)

simulate (*alphai*)

performs the actual reflectivity calculation for the specified incidence angles

Parameters

alphai: vector of incidence angles

Returns

vector of intensities of the reflectivity signal

xrayutilities.simpack.models.**startdelta** (*start*, *delta*, *num*)

xrayutilities.simpack.smaterials module

class xrayutilities.simpack.smaterials.**CrystalStack** (*name*, **args*)

Bases: **xrayutilities.simpack.smaterials.LayerStack**

extends the built in list type to enable building a stack of crystalline Layers by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**GradedLayerStack** (*alloy*, *xfrom*, *xto*, *nsteps*, *thickness*, ***kwargs*)

Bases: **xrayutilities.simpack.smaterials.CrystalStack**

generates a sequence of layers with a gradient in chemical composition

class xrayutilities.simpack.smaterials.**Layer** (*material*, *thickness*, ***kwargs*)

Bases: **xrayutilities.simpack.smaterials.SMaterial**

Object describing part of a thin film sample. The properties of a layer :are:

Material: an xrayutilties material describing optical and crystal properties of the thin film

Thickness: film thickness in Angstrom

Roughness: root mean square roughness of the top interface in Angstrom

class xrayutilities.simpack.smaterials.**LayerStack** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.MaterialList**
extends the built in list type to enable building a stack of Layer by various methods.

check (*v*)

class xrayutilities.simpack.smaterials.**MaterialList** (*name*, **args*)
Bases: **_abcoll.MutableSequence**
class representing the basics of a list of materials for simulations within xrayutilities. It extends the built in list type.

check (*v*)

insert (*i*, *v*)

class xrayutilities.simpack.smaterials.**PseudomorphicStack001** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.CrystalStack**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 001 and materials must be cubic/tetragonal.

insert (*i*, *v*)

make_epitaxial (*i*)

trans = *<xrayutilities.math.transforms.Transform object at 0x7f2db1e4ae50>*

class xrayutilities.simpack.smaterials.**PseudomorphicStack111** (*name*, **args*)
Bases: **xrayutilities.simpack.smaterials.PseudomorphicStack001**
generate a sequence of pseudomorphic crystalline Layers. Surface orientation is assumed to be 111 and materials must be cubic.

trans = *<xrayutilities.math.transforms.CoordinateTransform object at 0x7f2db0fe3090>*

class xrayutilities.simpack.smaterials.**SMaterial** (*material*, ***kwargs*)
Bases: **object**
Simulation Material. Extends the xrayutilities Materials by properties needed for simulations

Module contents

simulation subpackage of xrayutilities.

This package provides possibilities to simulate X-ray diffraction and reflectivity curves of thin film samples. It could be extended for more general use in future if there is demand for that.

In addition it provides a fitting routine for reflectivity data which is based on lmfit.

Submodules

xrayutilities.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.

xrayutilities.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)

Attibutes

expr -- input expression in which the error occurred :msg: -- explanation of the error

xrayutilities.experiment module

module helping with planning and analyzing experiments. various classes are provided for describing experimental geometries, calculationof angular coordinates of Bragg reflections, conversion of angular coordinates to Q-space and determination of powder diffraction peak positions.

The strength of the module is the versatile QConversion module which can be configured to describe almost any goniometer geometry.

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 Crystal. You can specify the matrix B (default identiy matrix) shape needs to be (3,3)

mat: Crystal 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

U: orientation matrix U can be given. If none is given the orientation defined in the Experiment class is used.

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

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

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

en: x-ray energy in eV (default: converted self._wl)

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

sampledis: sample displacement vector in relative units of the detector distance (default: (0, 0, 0))

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

q: list or numpy array with the reciprocal space position

optional keyword arguments:

deg: True/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. This is for example necessary before any Q2Ang-conversion can be performed.
Parameters

v: 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

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
Using this class the default sample surface orientation is determined by the inner most sample rotation (which is usually the azimuth motor).

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. However, if one angle is always the same its enough to give one scalar value.

****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)

deg: flag 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/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 [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.**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,beta: sample and detector angles as numpy array, lists or Scalars must be given. all arguments must have the same shape or length. Howevver, if one angle is always the same its enough to give one scalar value.

****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 3. Used angles are than ai,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)

deg: flag 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. However, if one angle is always the same its enough to give one scalar value.

****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)

deg: flag 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. The coplanar scattering angles correspond to a goniometer with sample rotations ['x+','y+','z-'] and detector rotation 'x+' and primary beam along y. This is a standard four circle diffractometer.

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/Flase (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 geometries return [omega,0,phi,twotheta]
- "realTilt" general geometry with angles determined by q-coordinates (tilt); returns [omega,chi,phi,twotheta]

default: self.geometry

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

mat: Crystal object; needed to obtain its optical properties for refraction correction, otherwise not used

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

fi,fd: if 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]

omega: incidence angle with respect to surface

chi: sample tilt for the case of non-coplanar geometry

phi: sample azimuth with respect to inplane reference direction

twotheta: scattering 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_i: offset of the incidence beam from the scattering plane due to refraction

pdi_d: offset ot 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,tt: sample and detector angles as numpy array, lists or Scalars must be given. All arguments must have the same shape or length. However, if one angle is always the same its enough to give one scalar value.

****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 om,chi,phi,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)

deg: flag 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/Flase (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*)

Convolutes 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 and X-ray energy. Both angular scans (where some goniometer angles change during data acquisition) and energy scans (where the energy is varied during acquisition) as well as mixed cases can be treated.
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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)

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

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

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

en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!

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

sampledis: sample displacement vector in same units as the detector distance (default: (0, 0, 0))

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 varing

detectorAxis
property handler for _detectorAxis
Returns
list of detector axis following the syntax /[xyz][+-]/

energy

getDetectorDistance (args*, ***kwargs*)**

obtains the detector distance by applying the detector arm movements. This is especially interesting for the case of 1 or 2D detectors to perform certain geometric corrections.
Parameters

***args: detector angles. Only detector arm angles as described by the**

detectorAxis attribute must be given.

****kwargs: optional keyword arguments**

dim: dimension of the detector for which the position should be determined

roi: region of interest for the detector pixels; :(default: self._area_roi/self._linear_roi)

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

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

Returns

numpy array with the detector distance

getDetectorPos (args*, ***kwargs*)**
obtains the detector position vector by applying the detector arm rotations.
Parameters

***args: detector angles. Only detector arm angles as described by the**

detectorAxis attribute must be given.

****kwargs: optional keyword arguments**

dim: dimension of the detector for which the position should be determined

roi: region of interest for the detector pixels; :(default: self._area_roi/self._linear_roi)

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

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

Returns

numpy array of length 3 with vector components of the detector direction. The length of the vector is k.

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

detectorDir1: direction of the detector (along the pixel direction 1); e.g. 'z+' means higher pixel numbers at larger z positions

detectorDir2: direction of the detector (along the pixel direction 2); e.g. 'x+'

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

Nch1: number of detector pixels along direction 1

Nch2: number 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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)

en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!

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

sampledis: sample displacement vector in same units as the detector distance (default: (0, 0, 0))

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 but can be mixed with Scalars (i.e. if an angle is always the same it can be given only once instead of an array)

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)

en: x-ray energy in eV (default is converted self._wl) both wavelength and energy can also be an array which enables the QConversion for energy scans. Note that the en keyword overrules the wl keyword!

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

sampledis: sample displacement vector in relative units of the detector distance (default: (0,0,0))

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][+-]/

transformSample2Lab (*vector*, **args*)

transforms a vector from the sample coordinate frame to the laboratory coordinate system by applying the sample rotations from inner to outer circle.
Parameters

vector: vector to transform (sequence, list, numpy array)

args: goniometer angles (sample angles or full goniometer angles can be given. If more angles than the sample circles are given they will be ignored)

Returns

rotated vector as numpy.array

wavelength

xrayutilities.gridder module

class xrayutilities.gridder.**FuzzyGridder1D** (*nx*)

Bases: **xrayutilities.gridder.Gridder1D**

An 1D binning class considering every data point to have a finite width. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite width (e.g. X-ray data from a 1D detector).

class xrayutilities.gridder.**Gridder**

Bases: **object**

Basis class for gridders in xrayutilities. A gridder is a function mapping irregular spaced data onto a regular grid by binning the data into equally sized elements.

There are different ways of defining the regular grid of a Gridder. In xrayutilities the data bins extend beyond the data range in the input data, but the given position being the center of these bins, extends from the minimum to the maximum of the data! The main motivation for this was to create a Gridder, which when feeded with N equidistant data points and gridded with N bins would not change the data position (not the case with numpy.histogramm functions!). Of course this leads to the fact that for homogeneous point density the first and last bin in any direction are not filled as the other bins.

A different definition is used by numpy histogram functions where the bins extend only to the end of the data range. (see numpy histogram, histrogram2d, ...)

Clear ()

Clear so far gridded data to reuse this instance of the Gridder

KeepData (*bool*)

Normalize (*bool*)

set or unset the normalization flag. Normalization needs to be done to obtain proper gridding but may want to be disabled in certain cases when sequential gridding is performed

data

return gridded data (performs normalization if switched on)

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

Bases: **xrayutilities.gridder.Gridder**

dataRange (*min*, *max*, *fixed=True*)

define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored

Parameters

min: minimum value of the gridding range

max: maximum value of the gridding range

fixed: flag to turn fixed range gridding on (True (default)) or off (False)

xaxis

Returns the xaxis of the gridder the returned values correspond to the center of the data bins used by the gridding algorithm

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.**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

class xrayutilities.gridder.**npyGridder1D** (*nx*)
Bases: **xrayutilities.gridder.Gridder1D**

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

xrayutilities.gridder2d module

class xrayutilities.gridder2d.**FuzzyGridder2D** (*nx*, *ny*)
Bases: **xrayutilities.gridder2d.Gridder2D**
An 2D binning class considering every data point to have a finite area. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite size (e.g. X-ray data from a 2D detector or reciprocal space maps measured with point/linear detector).
Currently only a rectangular area can be considered during the gridding.

class xrayutilities.gridder2d.**Gridder2D** (*nx*, *ny*)
Bases: **xrayutilities.gridder.Gridder**

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

dataRange (*xmin*, *xmax*, *ymin*, *ymax*, *fixed=True*)
define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored
Parameters

xmin,ymin: minimum value of the gridding range in x,y
xmax,ymax: maximum value of the gridding range in x,y
fixed: flag to turn fixed range gridding on (True (default)) or off (False)

xaxis

xmatrix

yaxis

ymatrix

class xrayutilities.gridder2d.**Gridder2DList** (*nx*, *ny*)
Bases: **xrayutilities.gridder2d.Gridder2D**
special version of a 2D gridder which performs no actual averaging of the data in one grid/bin but just collects the data-objects belonging to one bin for further treatment by the user

Clear ()

data
return gridded data, in this special version no normalization is defined!

xrayutilities.gridder3d module

class xrayutilities.gridder3d.**FuzzyGridder3D** (*nx*, *ny*, *nz*)
Bases: **xrayutilities.gridder3d.Gridder3D**
An 3D binning class considering every data point to have a finite volume. If necessary one data point will be split fractionally over different data bins. This is numerically more effort but represents better the typical case of a experimental data, which do not represent a mathematical point but have a finite size.
Currently only a quader can be considered as volume during the gridding.

class xrayutilities.gridder3d.**Gridder3D** (*nx*, *ny*, *nz*)
Bases: **xrayutilities.gridder.Gridder**

SetResolution (*nx*, *ny*, *nz*)

dataRange (*xmin*, *xmax*, *ymin*, *ymax*, *zmin*, *zmax*, *fixed=True*)
define minimum and maximum data range, usually this is deduced from the given data automatically, however, for sequential gridding it is useful to set this before the first call of the gridder. data outside the range are simply ignored
Parameters

xmin,ymin,zmin:	minimum value of the gridding range in x,y,z
xmax,ymax,zmax:	maximum value of the gridding range in x,y,z
fixed:	flag to turn fixed range gridding on (True (default)) or off (False)

xaxis

xmatrix

yaxis

ymatrix

zaxis

zmatrix

xrayutilities.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

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

Parameters

data: data which should be contracted (length N)

Nav: number 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

Parameters

data2d: array of 2D data shape (N,M)

Nav1,2: a field of (Nav1 x Nav2) values is contracted

****kwargs: optional keyword argument**

roi: region 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 serveral PSD spectra all data are used therefore the last cell used for averaging may differ in size
Parameters

psddata: array of 2D data shape (Nspectra,Nchannels)

Nav: number of channels which should be averaged

****kwargs: optional keyword argument**

roi: region 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))

xrayutilities.q2ang_fit module

Module provides functions to convert a q-vector from reciprocal space to angular space. a simple implementation uses scipy optimize routines to perform a fit for a arbitrary goniometer.

The user is, however, expected to use the bounds variable to put restrictions to the number of free angles to obtain reproducible results. In general only 3 angles are needed to fit an arbitrary q-vector (2 sample + 1 detector angles or 1 sample + 2 detector). More complicated restrictions can be implemented using the lmfit package. (done upon request!)

The function is based on a fitting routine. For a specific goniometer also analytic expressions from literature can be used as they are implemented in the predefined experimental classes HXRD, NonCOP, and GID.

Q2AngFit(qvec, expclass, bounds=None, ormat=array([[1., 0., 0.],
[0., 1., 0.],
[0., 0., 1.]]), startvalues=None, constraints=())

Functions to convert a q-vector from reciprocal space to angular space. This implementation uses scipy optimize routines to perform a fit for a goniometer with arbitrary number of goniometer angles.
The user *must* use the bounds variable to put restrictions to the number of free angles to obtain reproducible results. In general only 3 angles are needed to fit an arbitrary q-vector (2 sample + 1 detector angles or 1 sample + 2 detector).
Parameters

qvec: q-vector for which the angular positions should be calculated

expclass: experimental class used to define the goniometer for which the angles should be calculated.

keyword arguments(optional):

bounds: list of bounds of the goniometer angles. The number of bounds must correspond to the number of goniometer angles in the expclass. Angles can also be fixed by supplying only one value for a particular angle. e.g.: ((low, up), fix, (low2, up2), (low3, up3))

ormat: orientation matrix of the sample to be used in the conversion

startvalues: start values for the fit, which can significantly speed up the conversion. The number of values must correspond to the number of angles in the goniometer of the expclass

constraints: sequence of constraint dictionaries. This allows applying arbitrary (e.g. pseudo-angle) contraints by supplying according constraint functions. (see scipy.optimize.minimize). The supplied function will be called with the arguments (angles, qvec, Experiment, U).

Returns

fittedangles, qerror, errcode:

list of fitted goniometer angles, the error in reciprocal space and the errcode of the scipy minimize function. for a successful fit the error code should be <=2

xrayutilities.q2ang_fit.**exitAngleConst** (*angles*, *alphaf*, *hxrd*)
helper function for an pseudo-angle constraint for the Q2AngFit-routine.

Parameters

angles: fit parameters of Q2AngFit
alphaf: the exit angle which should be fixed
hxrd: the Experiment object to use for qconversion

xrayutilities.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)

Examples

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

xrayutilities.utilities_noconf module

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

`xrayutilities.utilities_noconf.`**`clear_bit`** (*`f`*, *`offset`*)
clears the bet at an offset

`xrayutilities.utilities_noconf.`**`en2lam`** (*`inp`*)
converts the input energy in eV to a wavelength in Angstrom
Parameters

inp: energy in eV

Returns

float, wavlength in Angstrom

Examples

```
>>> wavelength = en2lam(8048)
```

`xrayutilities.utilities_noconf.`**`energy`** (*`en`*)
convert common energy names to energies in eV
so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1
Parameters

en: energy either as scalar or array with value in eV, which will be returned unchanged; or string with name of emission line

Returns

energy in eV as float

`xrayutilities.utilities_noconf.`**`exchange_filepath`** (*`orig`*, *`new`*, *`keep=0`*)

function to exchange the root of a filename with the option of keeping the inner directory structure. This for example includes such a conversion /dir_a/subdir/sample/file.txt -> /home/user/data/sample/file.txt where the innermost directory name is kept (keep=1)
Parameters

orig: original filename which should have its data root replaced

new: new path which should be used instead

keep: (optional) number of inner most directory names which should be kept the same in the output (default = 0). Note that the filename is always return unchanged also with keep=0.

Returns

filename string

Examples

```
>>> exchange_filepath('/dir_a/subdir/sam/file.txt', '/data', 1)
'/data/sam/file.txt'
```

xrayutilities.utilities_noconf.**exchange_path** (*orig*, *new*, *keep=0*)
function to exchange the root of a path with the option of keeping the inner directory structure. This for example includes such a conversion /dir_a/subdir/images/sample -> /home/user/data/images/sample where the two innermost directory names are kept (keep=2)
Parameters

orig: original path which should be replaced by the new path

new: new path which should be used instead

keep: (optional) number of inner most directory names which should be kept the same in the output (default = 0)

Returns

directory path string

Examples

```
>>> exchange_path('/dir_a/subdir/img/sam', '/home/user/data', 2)
'/home/user/data/img/sam'
```

xrayutilities.utilities_noconf.**lam2en** (*inp*)
converts the input wavelength in Angstrom to an energy in eV
Parameters

inp: wavelength in Angstrom

Returns

float, energy in eV

Examples

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

xrayutilities.utilities_noconf.**set_bit** (*f*, *offset*)
sets the bit at an offset

xrayutilities.utilities_noconf.**wavelength** (*wl*)
convert common energy names to energies in eV
so far this works with CuKa1, CuKa2, CuKa12, CuKb, MoKa1
Parameters

wl: wavelength; If scalar or array the wavelength in Angstrom will be returned unchanged, string with emission name is converted to wavelength

Returns

wavelength in Angstrom as float

Module contents

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>

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