

CYXTAL

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Chapter 1

Namespace Index

1.1 Packages

Here are the packages with brief descriptions (if available):

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--	---

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

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cyxtal.cxtallite.Eulers	11
object	
cyxtal.ext_aps.parsers.VoxelStep	13
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Chapter 3

Class Index

3.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

cyxtal.cxtallite.Aggregate	11
cyxtal.cxtallite.Eulers	11
cyxtal.cxtallite.OrientationMatrix	12
cyxtal.cxtallite.Quaternion	12
cyxtal.cxtallite.Rodrigues	13
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cyxtal.cxtallite.Xtallite	17

Chapter 4

Namespace Documentation

4.1 cyxtal.ext_aps.parsers Namespace Reference

Classes

- class [VoxelStep](#)

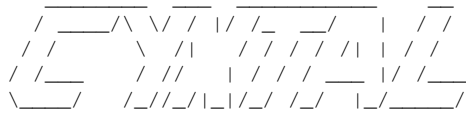
Functions

- def [parse_xml](#) (xmlfile, namespace={'step':'http://sector34.xor.aps.anl.gov/34ide:indexResult'}, disp=True)
- def [get_reciprocal_base](#) (lc, degrees=True)
- def [get_base](#) (lc, reciprocal=False, degrees=True)

Variables

- [theta_1](#) = -np.pi
MODULE LEVEL CONSTANTS RELATING TO COORDINATE TRANSFORMATION <NOTE> These are defined in terms of rotation matrices since it is more intuitive to see how each system is connected through simple rotation around x-axis (see cyxtal/documentation)
- **R_XHF2TSL**
- **R_TSL2XHF** = R_XHF2TSL.T
- float **theta_2** = -0.25
- **R_XHF2APS**
- **R_APS2XHF** = R_XHF2APS.T
- float **theta_3** = -0.75
- **R_APS2TSL**
- **R_TSL2APS** = R_APS2TSL.T
- **R_TSL2TSL** = np.eye(3)

4.1.1 Detailed Description



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DESCRIPTION

VoxelStep: class

Container class to store voxel information and perform strain refinement.

parser_xml: function

Parsing xml output from APS (with/without strain refinement).

get_reciprocal_base:

Return reciprocal basis according to given lattice constants.

get_base: function

Return lattice basis according to given lattice constants.

NOTE

More information regarding the coordinate transformation can be found at:

http://www.aps.anl.gov/Sectors/33_34/microdiff/Instrument/coordinates-PE-system.pdf

4.1.2 Function Documentation

4.1.2.1 `def cyxtal.ext_aps.parsers.get_base (lc, reciprocal=False, degrees=True)`

DESCRIPTION

basis = get_base(lc)

return the basis constructed based given lattice constant.

PARAMETERS

lc: numpy.array/list/tuple [a,b,c,alpha,beta,gamma]

Should contain necessary lattice constants that defines crystal structure.

reciprocal: boolean

Whether the returned basis vectors in real reciprocal space or real space.

degree: boolean

The angular lattice parameter are in degrees or radians.

RETURNS

rst: numpy.array

A 3x3 numpy array formed by the base vectors of given lattice constant. The base vectors are stack by column.

4.1.2.2 `def cyxtal.ext_aps.parsers.get_reciprocal_base (lc, degrees = True)`

DESCRIPTION

```
reciprocal_basis = get_reciprocal_base(lc)
    wrapper function to return the reciprocal basis rather
    than standard basis
```

PARAMETERS

```
lc: numpy.array/list/tuple [a,b,c,alpha,beta,gamma]
    Should contain necessary lattice constants that defines
    crystal structure.
degree: boolean
    The angular lattice parameter are in degrees or radians.
```

RETURNS

```
rst: numpy.array
    A 3x3 numpy array formed by the reciprocal base vectors of
    given lattice constant. The base vectors are stack by column.
```

4.1.2.3 `def cyxtal.ext_aps.parsers.parse_xml (xmlfile, namespace = {'step': 'http://sector34.xor.aps.anl.gov/34ide:indexResult'}, disp = True)`

DESCRIPTION

```
[VoxelStep(),...] = parse_xml(DAXM_DATA.xml,
                               namespace={XML_NAMESPACE_DICT},
                               disp=True)
```

Parse the DAXM data from Beamline 34-I-DE to memory.

PARAMETERS

```
xmlfile: str
    Path to the xml file requires data processing
namespace: dictionary
    Containing dictionary of the namespace used in the xml file.
    For data from beamline 34-ID-E, use the default setting should
    work.
NOTE:
    If the beamline changes there namespace, it is necessary to
    extract those namespace and update them with this argument.
```

```
disp: boolean
    Toggle output of parsing progress (terminal only)
```

RETURNS

```
voxels: list of VoxelStep
    List of instances of VoxelStep, each one representing indexed voxel
    in the xml data.
```

NOTE:

Not indexed file is screened out by checking the presence of a*
for each voxel.

NOTE

4.1.3 Variable Documentation

4.1.3.1 `cyxtal.ext_aps.parsers.R_APS2TSL`

Initial value:

```
1 = np.array([[1.0,          0.0,          0.0],
2             [0.0, np.cos(theta_3), -np.sin(theta_3)],
3             [0.0, np.sin(theta_3), np.cos(theta_3)]])
```

4.1.3.2 `cyxtal.ext_aps.parsers.R_XHF2APS`

Initial value:

```
1 = np.array([[1.0,          0.0,          0.0],
2             [0.0,  np.cos(theta_2), -np.sin(theta_2)],
3             [0.0,  np.sin(theta_2),  np.cos(theta_2)])])
```

4.1.3.3 `cyxtal.ext_aps.parsers.R_XHF2TSL`

Initial value:

```
1 = np.array([[1.0,          0.0,          0.0],
2             [0.0,  np.cos(theta_1), -np.sin(theta_1)],
3             [0.0,  np.sin(theta_1),  np.cos(theta_1)])])
```

4.1.3.4 `cyxtal.ext_aps.parsers.theta_1 = -np.pi`

MODULE LEVEL CONSTANTS RELATING TO COORDINATE TRANSFORMATION <NOTE> These are defined in terms of rotation matrices since it is more intuitive to see how each system is connected through simple rotation around x-axis (see `cyxtal/documentation`)

** XHF <-> TSL

Chapter 5

Class Documentation

5.1 `cyxtal.cxtallite.Aggregate` Class Reference

5.1.1 Detailed Description

```
DESCRIPTION
-----
grainX = Aggregate(ListOfXtallites)
    A container class that holds several
```

The documentation for this class was generated from the following file:

- `cxtallite.pyx`

5.2 `cyxtal.cxtallite.Eulers` Class Reference

5.2.1 Detailed Description

```
DESCRIPTION
-----
Euler angle representation of orientation.
Calculation is carries out by converting to quaternions.

PARAMETERS
-----
phi1: double
    first of Euler angle
PHI: double
    second of Euler angle
phi2: double
    third of Euler angle

METHODS
-----
```

The documentation for this class was generated from the following file:

- `cxtallite.pyx`

5.3 cyxtal.cxtallite.OrientationMatrix Class Reference

5.3.1 Detailed Description

Matrix representation of orientation, this is defined as the transpose of the rotation matrix.

PARAMETERS

METHODS

The documentation for this class was generated from the following file:

- cxtallite.pyx

5.4 cyxtal.cxtallite.Quaternion Class Reference

5.4.1 Detailed Description

DESCRIPTION

Quaternion(np.array([w,x,y,z]))

Quaternion is a set of numerics that extends from complex number, where a imaginary space (x,y,z) is constructed to facilitate a close set.

Particularly, the unitary quaternions correspond to the rotation operation in 3D space, which is why many computer graphics used it to perform fast rotation calculations.

PARAMETERS

q: DTYPE[:]

Simple vector with length 4

METHODS

unitary(self)

Return a unitary quaternion, useful for using quaternion to represent rotation/orientation.

conj(self)

Return the conjugate of the quaternion

tolist(self)

Return the quaternion as a simple python list

tondarray(self)

Return the quaternion as a numpy array (preferred)

toEulers(self)

Convert a unitary quaternion into Euler Angles (np.ndarray)

toRodrigues(self)

Convert a unitary quaternion into Rodrigue vector (np.ndarray)

toOrientationMatrix(self)

Convert a unitary quaternion into Orientation Matrix (np.ndarray)

CLASSMETHOD

scale(Quaternion q, DTYPE_t scalar)

Scale a quaternion vector with given scalar.

rotate(Quaternion q, DTYPE_t[:] pt)

Rotate pt around origin by q.

average(list qs)

Return an approximation of the average quaternion (forced to unitary) for qs (list of quaternions).

The documentation for this class was generated from the following file:

- cxtallite.pyx

5.5 cyxtal.cxtallite.Rodrigues Class Reference

5.5.1 Detailed Description

DESCRIPTION

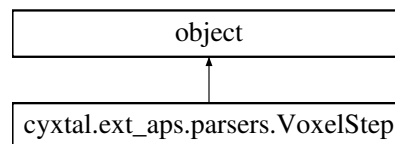
Rodrigues representation of orientation, a wrapper class that use Quaternion class as engine.

The documentation for this class was generated from the following file:

- cxtallite.pyx

5.6 cyxtal.ext_aps.parsers.VoxelStep Class Reference

Inheritance diagram for cyxtal.ext_aps.parsers.VoxelStep:



Public Member Functions

- def **__init__** (self)
- def **Xsample** (self)
- def **Xsample** (self, data)
- def **Ysample** (self)
- def **Ysample** (self, data)
- def **Zsample** (self)
- def **Zsample** (self, data)
- def **depth** (self)
- def **depth** (self, data)
- def **qs** (self)
- def **qs** (self, data)
- def **hkls** (self)
- def **hkls** (self, data)
- def **astar** (self)
- def **astar** (self, data)
- def **bstar** (self)
- def **bstar** (self, data)
- def **cstar** (self)
- def **cstar** (self, data)
- def **lc** (self)
- def **lc** (self, data)
- def **lattice** (self)
- def **lattice** (self, data)
- def **reciprocal_basis** (self)
- def **validate** (self, skip=False, tor=1e-2)

- `def __str__ (self)`
- `def get_coord (self, ref='TSL', translate=(0, 0, 0))`
- `def get_eulers (self, ref='TSL')`
- `def get_strain (self, ref='TSL', xtor=1e-8, disp=True, deviatoric=True, maxiter=1e4, weight=8e2, approximate=False, keep_volume=False)`
step 1: extract rotation (transformation).
- `def strain_refine (self, lc, r, weight)`
- `def strain_refine_tischler (self, lc, r, lattice_c)`

Public Attributes

- `qs`

5.6.1 Detailed Description

DESCRIPTION

Container class for parsing through data, all the data is stored as it is in the xml file. Additional methods are provided for various other purposes.

PARAMETERS

```

X|Y|Zsample:    sample motor position during scan (X|Y|Z)
depth:          wire position
qs:             identified diffraction vectors
hkls:           hkl indices identified
a|b|cstar:      strain free reciprocal lattice identified
lc:             lattice constants used in indexation
lattice:        lattice structure
_valid:         validation state of the voxel

```

5.6.2 Member Function Documentation

5.6.2.1 `def cyxtal.ext_aps.parsers.VoxelStep.get_coord (self, ref = 'TSL', translate = (0, 0, 0))`

DESCRIPTION

```

coord = self.get_coord(ref='TSL')
    Return the coordinates of the voxel in given reference
    system

```

PARAMETERS

```

ref: string(case insensitive)
    Name for reference configuration ['TSL'|'APS'|'XHF']
translate: array
    Translate voxel with given translation vector after
    rotating to the desired reference system.

```

NOTE

```

----
The rotation matrix and orientation matrix are a very confusing
couple, especially when it comes to crystallography. This is
most due to the fact both the crystal and the reference are constantly
transform during crystallography calculation. The general rule of thumb
in determine which matrix should be used should be as follows:
    if crystal.rotated is True & reference.rotated is False:
use Rotation_Matrix
    elif reference.rotated is True & crystal.rotated if False:
use Orientation_Matrix
    else:
call divide_and_couqure()
endif

```

5.6.2.2 `def cyxtal.ext_aps.parsers.VoxelStep.get_eulers (self, ref = 'TSL')`

DESCRIPTION

phil, PhH, phi2 = self.get_eulers(ref='TSL')

PARAMETERS

ref: string

The configuration in which the Euler Angles is computed.
 The default output (a*,b*,c*) in the xml file is in the
 APS coordinate system according to
http://www.aps.anl.gov/Sectors/33_34/microdiff/Instrument/coordinates-PE-system.pdf

RETURNS

phil, PHI, phi2: tuple

Computed Euler angles in degrees

NOTE

The change of reference configuration will affect the output
 of the Euler angle calculation, as a result, it is necessary
 define what configuration/reference the calculation is in and
 make sure all calculation is done under the same reference
 configuration.

5.6.2.3 `def cyxtal.ext_aps.parsers.VoxelStep.get_strain (self, ref = 'TSL', xtor = 1e-8, disp = True, deviatoric = True, maxiter = 1e4, weight = 8e2, approximate = False, keep_volume = False)`

step 1: extract rotation (transformation).

DESCRIPTION

epsilon = self.get_strain(ref='TSL')

Return strain tensor extracted/inferred through strain
 refinement process for current voxel. The returned strain
 tensor is transformed into designated coordinate system.

PARAMETERS

ref: str ['APS', 'TSL', XHF]

The coordinate system in which the refined strain tensor
 will be returned.

xtor: float

Tolerance used in the optimization of finding strained unit
 cell

disp: boolean

Toggle the display of optimization process results

deviatoric: boolean

Whether only returning the deviatoric strain components or
 full strain tensor

!!!NOTE:

Full strain tensor requires energy beam scan data,
 this particular feature has not implement yet.

maxiter: float

Maximum iterations/calls allowed during the optimization

weight: float

Fudge factor used to control the penalty term in the objective
 function of the optimization step (constrains on unit cell).

approximate: boolean

Perform full calculation of the residual strain tensor or using
 simple approximation $E = U - I$

keep_volume: boolean

Keep the volume to be constant throughout the strain refinement,
 which is suggested by Dr. Tischler at APS.

RETURNS

epsilon: np.array (3,3)

Strain tensor in given reference configuration

NOTE

Since the strain is approximated using the (a*,b*,c*), which are
 in the APS coordinate system.

step 2: call `scipy.optimize.minimize` on the objective function `self.get_qmismatch` to find the ideal set of lattice constants that provide best match to measured Q vectors. Since Dr.Tischler suggested a different approach, additional implementation is provided for this case. step 3: calculate the stretch tensor using the deformation gradient Dr. Tischler is doing all the calculation in the reciprocal space, however the deformation gradient is in real space. Based on the derivation in the reference, the ref: `cyxtal/documentation` step 4: transform strain tensor to requested configuration some preparation before hard computing

5.6.2.4 `def cyxtal.ext_aps.parsers.VoxelStep.qs (self, data)`

DESCRIPTION

Q vectors much be stack in rows, the xml file from aps are storing Q vectors by column.

5.6.2.5 `def cyxtal.ext_aps.parsers.VoxelStep.strain_refine (self, lc, r, weight)`

DESCRIPTION

`rst = self.strain_refine(lc, r, weight)`

This is the objective function for the strain refinement.

PARAMETERS

`lc: np.array`

lattice constant

`r: np.array (3,3)`

transformation matrix (orientation matrix) that converts standard unit cell system to APS coordinate system

`weight: float`

fudge factor in the penalty term that scales the effect of unit cell volume change

RETURNS

`rst: float`

angular difference between calculated qs using `new_lc` and measurements (`self.qs`). A penalty term (`delta_V`) is added to ensure no large strain happens to the unit cell.

NOTE

This approach is still under construction. Further change of the objective function is possible

5.6.2.6 `def cyxtal.ext_aps.parsers.VoxelStep.strain_refine_tischler (self, lc, r, lattice_c)`

Dr. Tischler implementation of strain refinement

NOTE:

This method currently leads to unstable results (singular matrix)

5.6.2.7 `def cyxtal.ext_aps.parsers.VoxelStep.validate (self, skip=False, tor=1e-2)`

DESCRIPTION

`self.validate()`

Validate all parameters are parsed;

Prune q vectors, ensure correct mapping between

`self.hkls` and `self.qs`;

Instance of `VoxelStep` can only be used when validated.

```

    If strain refinement is not required, set skip=True for
    quick data process.
PARAMETERS
-----
skip: boolean
    This flag allow a simple bypass of the type check that
    ensures all attributes are properly assigned.
tor: float
    Tolerance for q vectors pruning.
RETURNS
-----
self._valid: boolean
    Return the state of the voxel (valid/invalid)

```

The documentation for this class was generated from the following file:

- `ext_aps/parsers.py`

5.7 cyxtal.cxtallite.Xtallite Class Reference

5.7.1 Detailed Description

```

DESCRIPTION
-----
Composite class to represent material point in general crystal plasticity
simulation.

PARAMETERS
-----

METHODS
-----

```

The documentation for this class was generated from the following file:

- `cxtallite.pyx`

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- cyxtal.cxtallite.Eulers, [11](#)
- cyxtal.cxtallite.OrientationMatrix, [12](#)
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 - R_XHF2TSL, [10](#)
 - theta_1, [10](#)
- cyxtal::ext_aps::parsers::VoxelStep
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 - get_strain, [15](#)
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 - strain_refine_tischler, [16](#)
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- get_eulers
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- theta_1
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- validate
 - cyxtal::ext_aps::parsers::VoxelStep, [16](#)