

CYXTAL

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# Contents

<b>1</b>	<b>Namespace Index</b>	<b>1</b>
1.1	Packages	1
<b>2</b>	<b>Hierarchical Index</b>	<b>3</b>
2.1	Class Hierarchy	3
<b>3</b>	<b>Class Index</b>	<b>5</b>
3.1	Class List	5
<b>4</b>	<b>Namespace Documentation</b>	<b>7</b>
4.1	cyxtal.ext_aps.parsers Namespace Reference	7
4.1.1	Detailed Description	8
4.1.2	Function Documentation	8
4.1.2.1	get_base(lc, reciprocal=False, degrees=True)	8
4.1.2.2	get_reciprocal_base(lc, degrees=True)	9
4.1.2.3	parse_xml(xmlfile, namespace={'step':'http://sector34.xor.aps.anl.gov/34ide↵ :indexResult'}, disp=True)	9
4.1.3	Variable Documentation	9
4.1.3.1	R_APS2TSL	9
4.1.3.2	R_XHF2APS	10
4.1.3.3	R_XHF2TSL	10
4.1.3.4	theta_1	10

<b>5</b>	<b>Class Documentation</b>	<b>11</b>
5.1	cyxtal.cxtallite.Aggregate Class Reference	11
5.1.1	Detailed Description	11
5.2	cyxtal.cxtallite.Eulers Class Reference	11
5.2.1	Detailed Description	11
5.3	cyxtal.geometry.Line Class Reference	12
5.3.1	Detailed Description	12
5.3.2	Member Function Documentation	13
5.3.2.1	angle2line(self, other, inDegree=True)	13
5.3.2.2	contain_point(self, point)	13
5.3.2.3	dist2line(self, other)	13
5.3.2.4	dist2point(self, point)	13
5.3.2.5	get_intercept(self, other)	13
5.3.2.6	intercepted_by(self, other)	13
5.3.2.7	parallel_to(self, other)	14
5.3.2.8	skewed_from(self, other)	14
5.4	cyxtal.geometry.Line2D Class Reference	14
5.4.1	Detailed Description	15
5.4.2	Constructor & Destructor Documentation	15
5.4.2.1	__init__(self, pt_start, pt_end)	15
5.4.3	Member Function Documentation	15
5.4.3.1	get_discrete_pts(self, step=5)	15
5.4.3.2	get_intercept(self, other)	15
5.4.3.3	get_segments(self, step=5)	15
5.4.3.4	skewed_from(self, other)	15
5.5	cyxtal.cxtallite.OrientationMatrix Class Reference	16
5.5.1	Detailed Description	16
5.6	cyxtal.geometry.Plane Class Reference	16
5.6.1	Detailed Description	16
5.6.2	Member Function Documentation	17

5.6.2.1	<a href="#">contain_line(self, line)</a>	17
5.6.2.2	<a href="#">contain_point(self, point)</a>	17
5.6.2.3	<a href="#">normal(self)</a>	17
5.6.2.4	<a href="#">parallel_to(self, other)</a>	17
5.7	<a href="#">cxtal.geometry.Point Class Reference</a>	17
5.7.1	<a href="#">Detailed Description</a>	18
5.7.2	<a href="#">Member Function Documentation</a>	18
5.7.2.1	<a href="#">__str__(self)</a>	18
5.7.2.2	<a href="#">dist2line(self, line)</a>	18
5.7.2.3	<a href="#">dist2point(self, other)</a>	18
5.7.2.4	<a href="#">in_plane(self, plane)</a>	18
5.7.2.5	<a href="#">on_line(self, line)</a>	18
5.8	<a href="#">cxtal.geometry.Point2D Class Reference</a>	19
5.8.1	<a href="#">Detailed Description</a>	19
5.9	<a href="#">cxtal.geometry.Polygon2D Class Reference</a>	19
5.9.1	<a href="#">Detailed Description</a>	20
5.9.2	<a href="#">Constructor &amp; Destructor Documentation</a>	20
5.9.2.1	<a href="#">__init__(self)</a>	20
5.9.3	<a href="#">Member Function Documentation</a>	20
5.9.3.1	<a href="#">__str__(self)</a>	20
5.9.3.2	<a href="#">add_vertex(self, point)</a>	20
5.9.3.3	<a href="#">center(self)</a>	21
5.9.3.4	<a href="#">contains_point(self, point, ray_origin=None)</a>	21
5.9.3.5	<a href="#">get_shortest(self)</a>	21
5.10	<a href="#">cxtal.cxtallite.Quaternion Class Reference</a>	21
5.10.1	<a href="#">Detailed Description</a>	21
5.11	<a href="#">cxtal.cxtallite.Rodrigues Class Reference</a>	22
5.11.1	<a href="#">Detailed Description</a>	22
5.12	<a href="#">cxtal.ext_aps.parsers.VoxelStep Class Reference</a>	22
5.12.1	<a href="#">Detailed Description</a>	23
5.12.2	<a href="#">Member Function Documentation</a>	23
5.12.2.1	<a href="#">get_coord(self, ref='TSL', translate=(0, 0, 0))</a>	23
5.12.2.2	<a href="#">get_eulers(self, ref='TSL')</a>	24
5.12.2.3	<a href="#">get_strain(self, ref='TSL', xtor=1e-8, disp=False, deviatoric=True, maxiter=1e4, opt_method='nelder-mead')</a>	24
5.12.2.4	<a href="#">qs(self, data)</a>	25
5.12.2.5	<a href="#">strain_refine(self, v_features)</a>	25
5.12.2.6	<a href="#">validate(self, skip=False, tor=1e-2)</a>	25
5.13	<a href="#">cxtal.cxtallite.Xtallite Class Reference</a>	26
5.13.1	<a href="#">Detailed Description</a>	26



# Chapter 1

## Namespace Index

### 1.1 Packages

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

<a href="#">cyxtal.ext_aps.parsers</a> . . . . .	7
--	---





## Chapter 2

# Hierarchical Index

### 2.1 Class Hierarchy

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

cyxtal.cxtallite.Aggregate . . . . .	11
cyxtal.cxtallite.Eulers . . . . .	11
object	
cyxtal.ext_aps.parsers.VoxelStep . . . . .	22
cyxtal.geometry.Line . . . . .	12
cyxtal.geometry.Line2D . . . . .	14
cyxtal.geometry.Plane . . . . .	16
cyxtal.geometry.Point . . . . .	17
cyxtal.geometry.Point2D . . . . .	19
cyxtal.geometry.Polygon2D . . . . .	19
cyxtal.cxtallite.OrientationMatrix . . . . .	16
cyxtal.cxtallite.Quaternion . . . . .	21
cyxtal.cxtallite.Rodrigues . . . . .	22
cyxtal.cxtallite.Xtallite . . . . .	26



## Chapter 3

# Class Index

### 3.1 Class List

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

<a href="#">cyxtal.cxtallite.Aggregate</a>	11
<a href="#">cyxtal.cxtallite.Eulers</a>	11
<a href="#">cyxtal.geometry.Line</a>	12
<a href="#">cyxtal.geometry.Line2D</a>	14
<a href="#">cyxtal.cxtallite.OrientationMatrix</a>	16
<a href="#">cyxtal.geometry.Plane</a>	16
<a href="#">cyxtal.geometry.Point</a>	17
<a href="#">cyxtal.geometry.Point2D</a>	19
<a href="#">cyxtal.geometry.Polygon2D</a>	19
<a href="#">cyxtal.cxtallite.Quaternion</a>	21
<a href="#">cyxtal.cxtallite.Rodrigues</a>	22
<a href="#">cyxtal.ext_aps.parsers.VoxelStep</a>	22
<a href="#">cyxtal.cxtallite.Xtallite</a>	26



## Chapter 4

# Namespace Documentation

### 4.1 cyxtal.ext\_aps.parsers Namespace Reference

#### Classes

- class [VoxelStep](#)

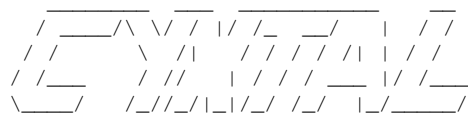
#### Functions

- 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](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

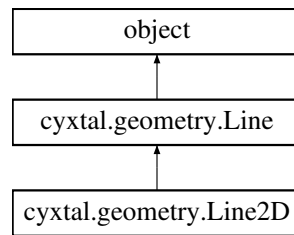
METHODS
-----
```

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

- `cxtallite.pyx`

## 5.3 cyxtal.geometry.Line Class Reference

Inheritance diagram for `cyxtal.geometry.Line`:



### Public Member Functions

- `def __init__ (self, pt_start, pt_end)`
- `def start_pt (self)`
- `def start_pt (self, new_start)`
- `def end_pt (self)`
- `def end_pt (self, new_end)`
- `def length (self)`
- `def direction (self)`
- `def __str__ (self)`
- `def __neg__ (self)`
- `def __eq__ (self, other)`
- `def __ne__ (self, other)`
- `def contain_point (self, point)`
- `def parallel_to (self, other)`
- `def skewed_from (self, other)`
- `def intercepted_by (self, other)`
- `def get_intercept (self, other)`
- `def dist2point (self, point)`
- `def dist2line (self, other)`
- `def angle2line (self, other, inDegree=True)`

### Public Attributes

- `start_pt`
- `end_pt`

#### 5.3.1 Detailed Description

DESCRIPTION

-----

`Line(Point pt_0, Point pt_1)`

A line(segment) in 3D space defined with 2 Point instances.

PARAMETERS

-----

`start_pt: Point`

Start point of the line instance.

`end_pt: Point`

End point of the line instance.

`length: float`

Return the length of the line segment.

```

direction: numpy.array
    Return the direction vector of the line segment.
    [start_pt->end_pt]
METHODS
-----
contain_point(Point pt)
    Test if self contains pt.
parallel_to(Line other)
    Test if self is parallel to other.
skewed_from(Line other)
    Test if self is skewed from other.
intercepted_by(Line other)
    Test if self is intercepted by other.
get_intercept(Line other)
    Return the intercept point.
dist2point(Point pt)
    Return the distance between self and pt (shortest).
dist2line(Line other)
    Return the distance between self and other (shortest).
angle2line(Line other, inDegree=True)
    Return the angle between self and other.
CLASSMETHOD
-----

```

### 5.3.2 Member Function Documentation

#### 5.3.2.1 `def cyxtal.geometry.Line.angle2line ( self, other, inDegree = True )`

Return angle between self and other

#### 5.3.2.2 `def cyxtal.geometry.Line.contain_point ( self, point )`

Test if self contains point

#### 5.3.2.3 `def cyxtal.geometry.Line.dist2line ( self, other )`

Return the distance between two skewed or parallel lines

#### 5.3.2.4 `def cyxtal.geometry.Line.dist2point ( self, point )`

Return the distance to a given point

#### 5.3.2.5 `def cyxtal.geometry.Line.get_intercept ( self, other )`

Return the intercept point if exist, or return None

#### 5.3.2.6 `def cyxtal.geometry.Line.intercepted_by ( self, other )`

Quick test if one line is intercepted by another

#### 5.3.2.7 `def cyxtal.geometry.Line.parallel_to ( self, other )`

Test if two Line are parallel to each other

#### 5.3.2.8 `def cyxtal.geometry.Line.skewed_from ( self, other )`

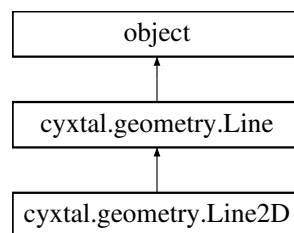
Quick test if one line is skewed from the other

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

- `geometry.py`

## 5.4 `cyxtal.geometry.Line2D` Class Reference

Inheritance diagram for `cyxtal.geometry.Line2D`:



### Public Member Functions

- `def \_\_init\_\_ (self, pt_start, pt_end)`
- `def \_\_str\_\_ (self)`
- `def direction (self)`
- `def parallel_to (self, other)`
- `def get\_intercept (self, other)`
- `def get\_discrete\_pts (self, step=5)`
- `def get\_segments (self, step=5)`

### Static Public Member Functions

- `def skewed\_from (self, other)`

## Additional Inherited Members

### 5.4.1 Detailed Description

```

DESCRIPTION
-----
Line2D(Point2D pt_start, Point2D pt_end)
    A 2D line (derived from the 3D Line class).
PARAMETERS
-----
METHODS
-----
get_discrete_pts(step=5)
    Return a numpy.array of coordinates discretize the 2D line.
get_segments(step=5)
    Return a numpy.array of segments.
CLASSMETHOD
-----

```

### 5.4.2 Constructor & Destructor Documentation

#### 5.4.2.1 `def cyxtal.geometry.Line2D.__init__( self, pt_start, pt_end )`

Using two 2D point to define a 2D line

### 5.4.3 Member Function Documentation

#### 5.4.3.1 `def cyxtal.geometry.Line2D.get_discrete_pts( self, step = 5 )`

return a list of coordinates discretize the line

#### 5.4.3.2 `def cyxtal.geometry.Line2D.get_intercept( self, other )`

Return the intercept of two lines

#### 5.4.3.3 `def cyxtal.geometry.Line2D.get_segments( self, step = 5 )`

return a list of segments

#### 5.4.3.4 `def cyxtal.geometry.Line2D.skewed_from( self, other ) [static]`

2D lines do not skew from each other

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

- geometry.py

## 5.5 cyxtal.cxtallite.OrientationMatrix Class Reference

### 5.5.1 Detailed Description

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

PARAMETERS

-----

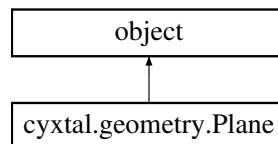
METHODS

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

- cxtallite.pyx

## 5.6 cyxtal.geometry.Plane Class Reference

Inheritance diagram for cyxtal.geometry.Plane:



### Public Member Functions

- def **\_\_init\_\_** (self, point1, point2, point3)
- def **normal** (self)
- def **\_\_str\_\_** (self)
- def **\_\_eq\_\_** (self, other)
- def **contain\_point** (self, point)
- def **contain\_line** (self, line)
- def **parallel\_to** (self, other)

### 5.6.1 Detailed Description

DESCRIPTION

-----

Plane(Point pt\_1, Point pt\_2, Point pt\_3)  
A plane in 3D space defined with 3 points.

PARAMETERS

-----

pt\_0, pt\_1, pt\_2: Point  
Three non collinear points defines the flat plane (self).  
normal: numpy.array  
Plane normal

METHODS

-----

contain\_point(Point point)  
Test if self contains pt.  
contain\_line(Line l)  
Test if self contains l.  
parallel\_to(Plane other)  
Test if self and other are parallel to each other.

CLASSMETHOD

-----

## 5.6.2 Member Function Documentation

### 5.6.2.1 `def cyxtal.geometry.Plane.contain_line ( self, line )`

Quick test to see if a line lies in a plane

### 5.6.2.2 `def cyxtal.geometry.Plane.contain_point ( self, point )`

Quick test to see if a point is in plane

### 5.6.2.3 `def cyxtal.geometry.Plane.normal ( self )`

Plane normal

### 5.6.2.4 `def cyxtal.geometry.Plane.parallel_to ( self, other )`

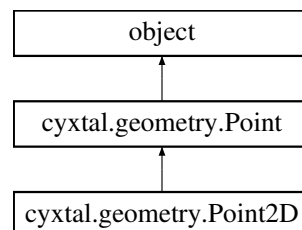
Quick test if two planes are parallel to each other

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

- geometry.py

## 5.7 cyxtal.geometry.Point Class Reference

Inheritance diagram for `cyxtal.geometry.Point`:



### Public Member Functions

- `def __init__ (self, x, y, z)`
- `def x (self)`
- `def x (self, val)`
- `def y (self)`
- `def y (self, val)`
- `def z (self)`
- `def z (self, val)`
- `def coord (self)`
- `def coord (self, val)`
- `def __str__ (self)`
- `def __eq__ (self, other)`
- `def __ne__ (self, other)`
- `def __len__ (self)`
- `def dist2point (self, other)`
- `def dist2line (self, line)`
- `def on_line (self, line)`
- `def in_plane (self, plane)`

### 5.7.1 Detailed Description

```

DESCRIPTION
-----
Point(x,y,z)
    Point in 3D space, base class provide bare bone abstraction
    for point related calculation.
PARAMETERS
-----
x,y,z: float
    Standard Cartesian coordinates for location description.
coord: array
    Vector of the Cartesian coordinates.
METHODS
-----
dist2point(Point other)
    Return the distance to another instance of Point.
dist2line(Line other)
    Return the distance to given instance of Line.
on_line(Line other)
    Whether the current instance lies on a given instance of Line.
in_plane(Plane other)
    Whether the current point lies in a given instance of Plane.
CLASSMETHOD
-----

```

### 5.7.2 Member Function Documentation

#### 5.7.2.1 `def cyxtal.geometry.Point.__str__( self )`

String representation of Point

#### 5.7.2.2 `def cyxtal.geometry.Point.dist2line ( self, line )`

Return the distance to another line

#### 5.7.2.3 `def cyxtal.geometry.Point.dist2point ( self, other )`

Return the distance to another point

#### 5.7.2.4 `def cyxtal.geometry.Point.in_plane ( self, plane )`

Quick test if a point is in a given plane

#### 5.7.2.5 `def cyxtal.geometry.Point.on_line ( self, line )`

Quick test is the point is on the given line

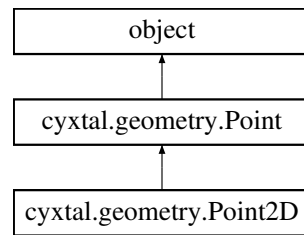
The documentation for this class was generated from the following file:

- geometry.py



## 5.8 cyxtal.geometry.Point2D Class Reference

Inheritance diagram for cyxtal.geometry.Point2D:



### Public Member Functions

- `def __init__(self, x, y)`
- `def __len__(self)`
- `def __str__(self)`

### 5.8.1 Detailed Description

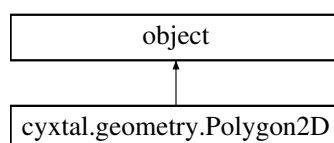
```
DESCRIPTION
-----
Point2D(x,y)
    A 2D point (derived from the 3D Point class).
PARAMETERS
-----
METHODS
-----
CLASSMETHOD
-----
```

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

- `geometry.py`

## 5.9 cyxtal.geometry.Polygon2D Class Reference

Inheritance diagram for cyxtal.geometry.Polygon2D:



## Public Member Functions

- def `__init__` (self)
- def `__str__` (self)
- def `edges` (self)
- def `vertices` (self)
- def `center` (self)
- def `add_vertex` (self, point)
- def `get_shortest` (self)
- def `contains_point` (self, point, ray\_origin=None)

### 5.9.1 Detailed Description

```

DESCRIPTION
-----
Polygon2D()
    A 2D polygon class.
PARAMETERS
-----
edges: list
    List of segments/edges of the 2D polygon.
vertices: list
    List of 2D points serve as the vertices of the 2D polygon.
center: Point2D
    Gravity center of the polygon.
METHODS
-----
add_vertex(Point new_vtx)
    Add new vertex to self.
get_shortest()
    Return the shortest distance between the center and vertices.
contains_point(Point point, ray_origin=None)
    Test if given point lies inside self.
CLASSMETHOD
-----

```

### 5.9.2 Constructor & Destructor Documentation

#### 5.9.2.1 def cyxtal.geometry.Polygon2D.\_\_init\_\_( self )

Initialize a 2D polygon with empty vertices list

### 5.9.3 Member Function Documentation

#### 5.9.3.1 def cyxtal.geometry.Polygon2D.\_\_str\_\_( self )

Formatted output for 2D polygon

#### 5.9.3.2 def cyxtal.geometry.Polygon2D.add\_vertex( self, point )

Add one more vertex to the current Polygon

**5.9.3.3** `def cyxtal.geometry.Polygon2D.center ( self )`

return the gravity center

**5.9.3.4** `def cyxtal.geometry.Polygon2D.contains_point ( self, point, ray_origin=None )`

quick test if a Point2D instance is inside the polygon.

**5.9.3.5** `def cyxtal.geometry.Polygon2D.get_shortest ( self )`

return the shortest distance between the center and vertices

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

- geometry.py

**5.10 cyxtal.cxtallite.Quaternion Class Reference****5.10.1 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

## 5.11 cyxtal.cxtallite.Rodrigues Class Reference

### 5.11.1 Detailed Description

#### DESCRIPTION

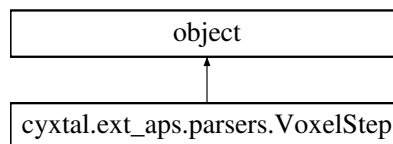
Rodrigues representation of orientation, a wrapper class that use Quaternion class as engine.

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

- cxtallite.pyx

## 5.12 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 **goodness** (self)
- def **goodness** (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=False, deviatoric=True, maxiter=1e4, opt\_method='nelder-mead')
  - step 4: transform strain tensor to requested configuration some preparation before hard computing*
- def **strain\_refine** (self, v\_features)

## Public Attributes

- **qs**

### 5.12.1 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  
 hkl: hkl indices identified  
 a|b|cstar: strain free reciprocal lattice identified  
 lc: lattice constants used in indexation  
 lattice: lattice structure  
 goodness: the indexation goodness of first pattern (highest confidence)  
 \_valid: validation state of the voxel

### 5.12.2 Member Function Documentation

#### 5.12.2.1 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

### 5.12.2.2 `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](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.

### 5.12.2.3 `def cyxtal.ext_aps.parsers.VoxelStep.get_strain ( self, ref = 'TSL', xtor = 1e-8, disp = False, deviatoric = True, maxiter = 1e4, opt_method = 'nelder-mead' )`

step 4: transform strain tensor to requested configuration some preparation before hard computing

#### 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

#### RETURNS

-----

epsilon: np.array (3,3)

Green--Lagrange strain tensor in given reference configuration

#### NOTE

----

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

5.12.2.4 `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.

5.12.2.5 `def cyxtal.ext_aps.parsers.VoxelStep.strain_refine( self, v_features )`

## DESCRIPTION

-----

```
rst = self.strain_refine(v_features)
    This is the objective function for the strain refinement.
```

## PARAMETERS

-----

```
v_features: np.array
    feature vectors
    (a*_1, a*_2, a*_3, b*_1, b*_2, b*_3, c*_1, c*_2, c*_3)
```

## RETURNS

-----

```
rst: float
    1-cos(q_calc, q_meas).
```

## NOTE

-----

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

5.12.2.6 `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`

## 5.13 cyxtal.cxtallite.Xtallite Class Reference

### 5.13.1 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



# Index

- `__init__`
    - `cyxtal::geometry::Line2D`, [15](#)
    - `cyxtal::geometry::Polygon2D`, [20](#)
  - `__str__`
    - `cyxtal::geometry::Point`, [18](#)
    - `cyxtal::geometry::Polygon2D`, [20](#)
- `add_vertex`
  - `cyxtal::geometry::Polygon2D`, [20](#)
- `angle2line`
  - `cyxtal::geometry::Line`, [13](#)
- `center`
  - `cyxtal::geometry::Polygon2D`, [20](#)
- `contain_line`
  - `cyxtal::geometry::Plane`, [17](#)
- `contain_point`
  - `cyxtal::geometry::Line`, [13](#)
  - `cyxtal::geometry::Plane`, [17](#)
- `contains_point`
  - `cyxtal::geometry::Polygon2D`, [21](#)
- `cyxtal.cxtallite.Aggregate`, [11](#)
- `cyxtal.cxtallite.Eulers`, [11](#)
- `cyxtal.cxtallite.OrientationMatrix`, [16](#)
- `cyxtal.cxtallite.Quaternion`, [21](#)
- `cyxtal.cxtallite.Rodrigues`, [22](#)
- `cyxtal.cxtallite.Xtallite`, [26](#)
- `cyxtal.ext_aps.parsers`, [7](#)
- `cyxtal.ext_aps.parsers.VoxelStep`, [22](#)
- `cyxtal.geometry.Line`, [12](#)
- `cyxtal.geometry.Line2D`, [14](#)
- `cyxtal.geometry.Plane`, [16](#)
- `cyxtal.geometry.Point`, [17](#)
- `cyxtal.geometry.Point2D`, [19](#)
- `cyxtal.geometry.Polygon2D`, [19](#)
- `cyxtal::ext_aps::parsers`
  - `get_base`, [8](#)
  - `get_reciprocal_base`, [8](#)
  - `parse_xml`, [9](#)
  - `R_APS2TSL`, [9](#)
  - `R_XHF2APS`, [9](#)
  - `R_XHF2TSL`, [10](#)
  - `theta_1`, [10](#)
- `cyxtal::ext_aps::parsers::VoxelStep`
  - `get_coord`, [23](#)
  - `get_eulers`, [23](#)
  - `get_strain`, [24](#)
  - `qs`, [24](#)
  - `strain_refine`, [25](#)
  - `validate`, [25](#)
- `cyxtal::geometry::Line`
  - `angle2line`, [13](#)
  - `contain_point`, [13](#)
  - `dist2line`, [13](#)
  - `dist2point`, [13](#)
  - `get_intercept`, [13](#)
  - `intercepted_by`, [13](#)
  - `parallel_to`, [13](#)
  - `skewed_from`, [14](#)
- `cyxtal::geometry::Line2D`
  - `__init__`, [15](#)
  - `get_discrete_pts`, [15](#)
  - `get_intercept`, [15](#)
  - `get_segments`, [15](#)
  - `skewed_from`, [15](#)
- `cyxtal::geometry::Plane`
  - `contain_line`, [17](#)
  - `contain_point`, [17](#)
  - `normal`, [17](#)
  - `parallel_to`, [17](#)
- `cyxtal::geometry::Point`
  - `__str__`, [18](#)
  - `dist2line`, [18](#)
  - `dist2point`, [18](#)
  - `in_plane`, [18](#)
  - `on_line`, [18](#)
- `cyxtal::geometry::Polygon2D`
  - `__init__`, [20](#)
  - `__str__`, [20](#)
  - `add_vertex`, [20](#)
  - `center`, [20](#)
  - `contains_point`, [21](#)
  - `get_shortest`, [21](#)
- `dist2line`
  - `cyxtal::geometry::Line`, [13](#)
  - `cyxtal::geometry::Point`, [18](#)
- `dist2point`
  - `cyxtal::geometry::Line`, [13](#)
  - `cyxtal::geometry::Point`, [18](#)
- `get_base`
  - `cyxtal::ext_aps::parsers`, [8](#)
- `get_coord`
  - `cyxtal::ext_aps::parsers::VoxelStep`, [23](#)
- `get_discrete_pts`
  - `cyxtal::geometry::Line2D`, [15](#)
- `get_eulers`
  - `cyxtal::ext_aps::parsers::VoxelStep`, [23](#)
- `get_intercept`

- cyxtal::geometry::Line, [13](#)
  - cyxtal::geometry::Line2D, [15](#)
- get\_reciprocal\_base
  - cyxtal::ext\_aps::parsers, [8](#)
- get\_segments
  - cyxtal::geometry::Line2D, [15](#)
- get\_shortest
  - cyxtal::geometry::Polygon2D, [21](#)
- get\_strain
  - cyxtal::ext\_aps::parsers::VoxelStep, [24](#)
- in\_plane
  - cyxtal::geometry::Point, [18](#)
- intercepted\_by
  - cyxtal::geometry::Line, [13](#)
- normal
  - cyxtal::geometry::Plane, [17](#)
- on\_line
  - cyxtal::geometry::Point, [18](#)
- parallel\_to
  - cyxtal::geometry::Line, [13](#)
  - cyxtal::geometry::Plane, [17](#)
- parse\_xml
  - cyxtal::ext\_aps::parsers, [9](#)
- qs
  - cyxtal::ext\_aps::parsers::VoxelStep, [24](#)
- R\_APS2TSL
  - cyxtal::ext\_aps::parsers, [9](#)
- R\_XHF2APS
  - cyxtal::ext\_aps::parsers, [9](#)
- R\_XHF2TSL
  - cyxtal::ext\_aps::parsers, [10](#)
- skewed\_from
  - cyxtal::geometry::Line, [14](#)
  - cyxtal::geometry::Line2D, [15](#)
- strain\_refine
  - cyxtal::ext\_aps::parsers::VoxelStep, [25](#)
- theta\_1
  - cyxtal::ext\_aps::parsers, [10](#)
- validate
  - cyxtal::ext\_aps::parsers::VoxelStep, [25](#)