Simulation of CXRS spectra using Raysect and CHERAB frameworks

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Contents

1 Purpose

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2 Scope

This document is applicable to the 55.EC CXRS Edge diagnostic. The CXRS Edge system is an optical diagnostic that collects the light emitted by the plasma upon interaction with the Diagnostic Neutral Beam (DNB) and analyses this light to extract the ion temperature, plasma rotation velocities and impurity content of the plasma. An overview of the CXRS Edge system is given in the Design Description document (DDD) [1].

3 Definitions

For a complete list of ITER abbreviations see [2]. Below abbreviations used in this document are given.

CXRS	Charge eXchange Recombination Spectroscopy
DNB	Diagnostic Neutral Beam

4 Introduction

4.1 CXRS Diagnostics

4.1.1 CXRS for Plasma Measurements

The Charge Exchange Recombination Spectroscopy (CXRS) diagnostics measures line emissions of several impurity isotopes in the plasma excited by charge exchange reactions with neutral hydrogen atoms injected into the plasma by the diagnostic neutral beam (DNB) (eqs. (1) and (2)). This line emission (table 1) provides essential information for plasma control and physics studies: ion temperature T_i (eq. (3)), toroidal (v_{tor}) and poloidal (v_{pol}) plasma rotation velocity (eq. (4)), helium ash and low Z impurity densities (beryllium, carbon, neon etc.) and the derived quantities such as Z_{eff} (eq. (5)).

$$X^{Z+} + H^0 \rightarrow X^{(Z-1)+}(n_2) + H^+ \tag{1}$$

$$X^{(Z-1)+}(n_2) \rightarrow X^{(Z-1)+}(n_1) + h\nu \tag{2}$$

$$kT_{\text{ion}} = mc^2 \frac{\Delta\lambda^2_{\text{Dopp}}}{\lambda_0^2} \tag{3}$$

where k – Boltzmann constant, $\Delta\lambda_{\text{dopp}}$ – line's width due to Doppler broadening, λ_0 – "natural", unshifted wavelength of the line's center.

$$v_{\text{rot}} = c \frac{\Delta\lambda_{\text{rot}}}{\lambda_0 \cos\alpha} \tag{4}$$

where $\Delta\lambda_{\text{rot}}$ – line's shift due to Doppler effect, α – angle between line of sight and toroidal direction.

$$n_{\text{imp}} = \frac{4\pi \int I(\lambda)\, d\lambda}{n_{\text{b}} Q^{\text{eff}}_{\text{CX}}(v_{\text{b}})\, dl} \tag{5}$$

where $I(\lambda)$ – intensity of the line, n_{b} – local neutral beam density, $Q^{\text{eff}}_{\text{CX}}(v_{\text{b}})$ – effective rate coefficient due to charge exchange, l – coordinate along a line of sight.

4.1.2 CXRS in ITER

The CXRS Edge diagnostic is a distributed system with components throughout the ITER tokamak complex. The primary viewing components (front-end optics) are installed in Equatorial port 3 (EP3), viewing the Diagnostic Neutral Beam (DNB) that enters the plasma in the neighboring section 4. Front-end optics consists of two light collecting systems: Upper and Lower. The scope of the 55.EC CXRS Edge diagnostic for Upper system ends at the image plane in the port interspace (11-L1-C03) where the collected signal is coupled into optical fibre bundles.

Table 1. Spectroscopic lines used in CXRS.

Ion	Transition	Wavelength
BeIV	$6 \rightarrow 5$	465.8 nm
BeIV	$8 \rightarrow 6$	468.5 nm
HeII	$4 \rightarrow 3$	468.5 nm
ArXVIII	$16 \rightarrow 15$	522.5 nm
NeX	$11 \rightarrow 10$	524.9 nm
CVI	$8 \rightarrow 7$	529.1 nm
Hα		656.3 nm
MSE		659.1 nm

For Lower system, however, 55.EC CXRS Edge diagnostic is responsible for light collection system, light transportation and detection. The collected signal is transported through optical fibre bundles to the Tritium building (Building 14 – Level 2 – Room 4), where the detection systems are located.

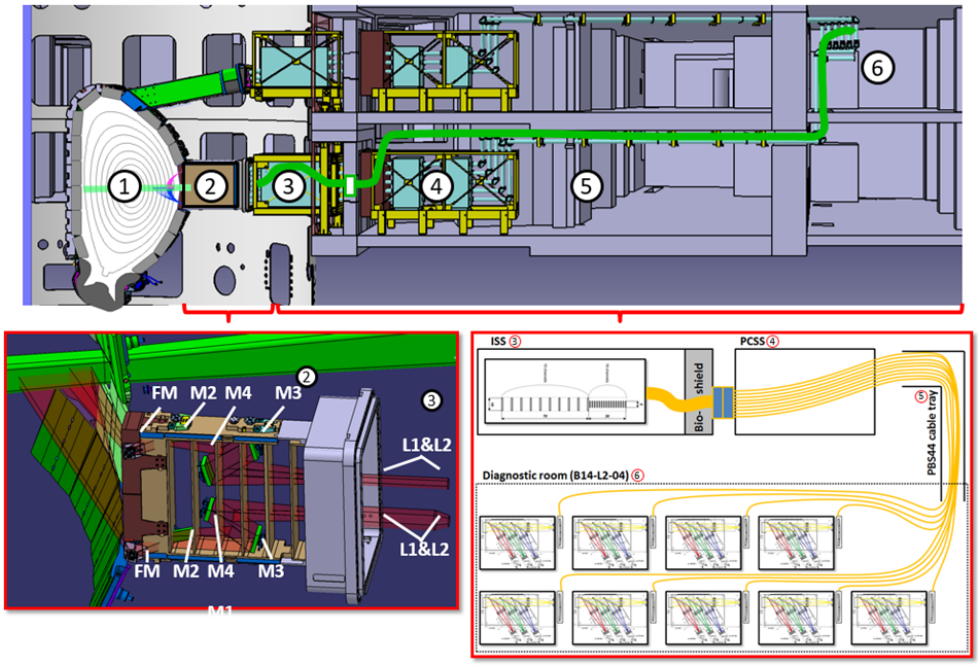

Figure 1. An overview of the CXRS Edge diagnostic design.

4.2 Development of the New Simulation Code

4.2.1 Existing Code

Simulation of Spectra (SOS) code by M. G. von Hellermann [3]

Features:

- Simulation takes into account many physical effects (halo effect, crossection effect, plume effect and others);
- Written in Matlab;
- Has Graphical User Interface (fig. 2).

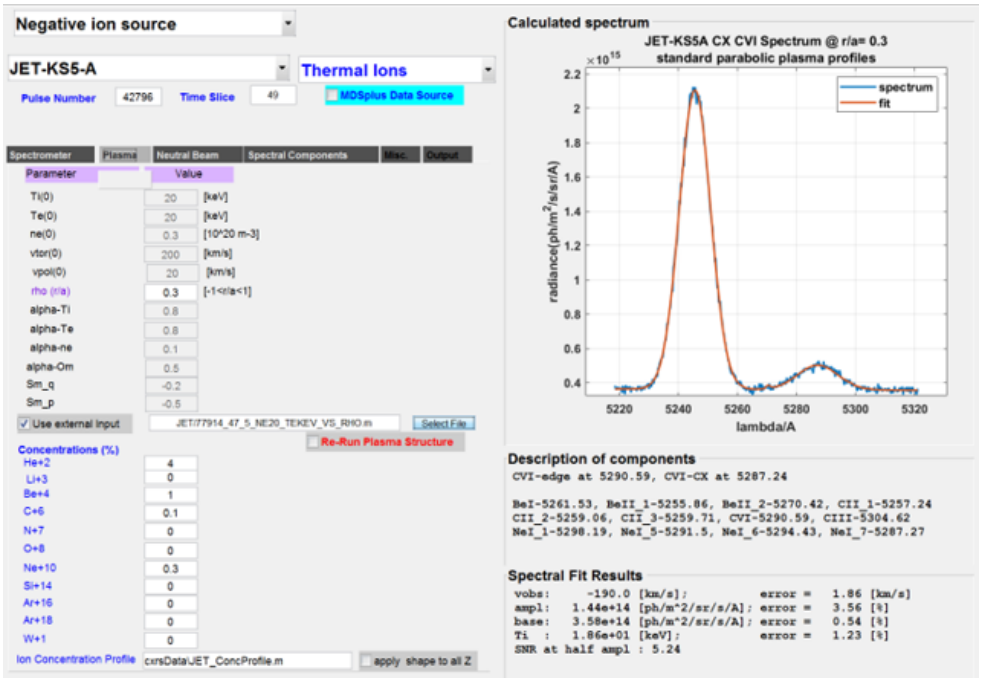

Figure 2. SOS interface.

4.2.2 Motivation

Existing code (Simulation of Spectra – SOS) lacks some features:

- Simplified plasma, tokamak and diagnostic geometry (e.g. elliptical plasma, point emission and others);
- Does not take reflections into account;
- Cannot use data from IMAS directly;
- Requires Matlab license, hard to extend by new developers.

The goal was to create an open and extensible simulation code using Python.

Sub goals:

- Implement interaction with IMAS database (read and write);
- Use IMAS data to create a plasma and diagnostic beam with spatial distributions;
- Use a ray-tracing engine to simulate spectra, this includes how reflections affect simulated spectra;
- Ensure that emission models include all physics already captured by SOS.

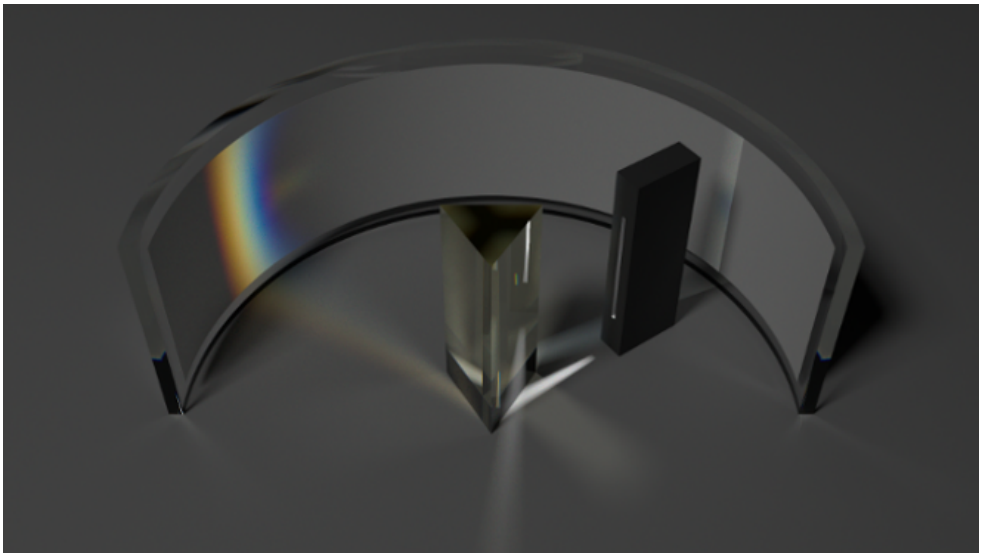

Figure 3. Demonstration of Raysect features.

4.3 Raysect and CHERAB

Raysect [4] is a ray-tracing framework for Python designed for scientific purposes.

- Supports scientific ray-tracing of spectra from physical light sources such as plasmas.
- Easily extensible, written with user customisation of materials and emissive sources in mind.
- Different observer types supported such as pinhole cameras and optical fibres.

CHERAB [5] is a Python library for forward modelling diagnostics based on spectroscopic plasma emission which provides physical models for Raysect. Provided models for Raysect:

- Tools for plasma and diagnostic beam simulations;
- Physical emission models (active charge exchange, bremsstrahlung and more).

5 Simulation of CXRS Spectra

Main part

6 Conclusion

Conclusion

References

[1] Zvonkov A., Serov S., and Tugarinov S. *System Design Description (DDD) 55.EC CXRS Edge*. Version 4.1. Apr. 2020.

[2] *ITER Abbreviations*. Version 1.17. Mar. 2018.

[3] Manfred von Hellermann et al. “Simulation of Spectra Code (SOS) for ITER Active Beam Spectroscopy”. In: *Atoms* 7.1 (Mar. 2019), p. 30. DOI: 10.3390/atoms7010030.

[4] Dr Alex Meakins and Matthew Carr. *raysect/source: v0.5.2 Release*. Version v0.5.2. Aug. 2018. DOI: 10.5281/zenodo.1341376. URL: https://doi.org/10.5281/zenodo.1341376.

[5] Dr Carine Giroud et al. *CHERAB Spectroscopy Modelling Framework*. Version v0.1.0. Mar. 2018. DOI: 10.5281/zenodo.1206142. URL: https://doi.org/10.5281/zenodo.1206142.

Appendices

A For Users

A.1 Installation

Clone this repository then go to its root folder:

```
git clone ssh://git@git.iter.org/diag/cxrs.git
cd cxrs
```

First of all you have to load all required modules:

```
source env.sh
```

This will purge all loaded modules and load ones that necessary to install and use `cxrs`.
To install `cxrs` on your computer run

```
pip install --user .
```

while in the the `cxrs` root directory.

Note: you can omit `python -m` part later by adding `$HOME/.local/bin` to your `PATH`. To do so, locate file `.bashrc` in your home directory and add the following line at the end of the file:

```
export PATH="$PATH:/home/ITER/<username>/.local/bin"
```

where `<username>` is your username at ITER GPC. You can look at it by executing next command via command line: `echo $USER`.

A.2 Preparations for the first run

Step 1: Create environment file

In order to create environment file, run

```
python -m cxrs create-env
```

This will create the default environment file, that loads all needed modules. To do so, run

```
source env.sh
```

It will purge all loaded modules and will load modules necessary to use `cxrs`.

Note: you have to do this for every new session on ITER GPC.

Step 2: Create configuration file

`cxrs` behavior controlled by configuration file which is necessary to run the code.

To create default configuration file, run

```
python -m cxrs create-config
```

This will create a configuration file with a name `config.xml` in current directory.

Step 3: Populate local atomic database

`cxrs` uses a local atomic database. To create one, run

```
python -m cxrs populate
```

Atomic data will be copied to the `$HOME/.cherab` directory.

A.3 Usage

A.3.1 Performing a simulation

Main part of `cxrs` is simulation routine, to use it for pulse with `<shot>` shot number and `<run>` run number for time slice `<time>` use:

```
python -m cxrs simulate -s <shot> -r <run> -t <time> -c <config>
```

where `<config>` is a path to configuration file.

It will perform a simulation and will store result in newly created folder `cxrs_output`.

Note: `time` can be omitted. In that case time slice in the middle of the time range will be used. This is particularly useful for time slices with a lot of digits after after decimal separator. For example :

```
python -m cxrs simulate -s 134000 -r 30 -c config.xml
```

For additional information use help:

```
python -m cxrs simulate --help
```

A.3.2 Print plasma profiles

`cxrs info` subprogram can be used to inspect different distributions of plasma and DNB parameters. To use it, run

```
python -m cxrs info -s <shot> -r <run>
```

It will produce variety of plots and tables and place it in `cxrs_output` folder. *Note:* 1D profiles represent values at the DNB axis.

A.3.3 Print plasma composition

You can quickly look at plasma composition for requested pulse by using

```
python -m cxrs composition -s <shot> -r <run>
```

Omit arguments to print composition for all pulses available by `scenario_summary` program.

A.3.4 Configuration

`cxrs` accepts user's configurations as xml-file.

To change option's value, change value attribute in double quotes corresponding to the option.

For more information on the meaning of certain parameter, look at its description.

Note: type attribute is actually important. For string values use `str`, for floating-point values use `float` and `int` for integers.

Warning: Do not change tags, like `<user_options>` or others, this will stop the program from working.

A.3.5 Emission parameters

Section `emission_parameters` controls which emission types are used during a simulation. Each of them can be turned on or off separately.

A.3.6 Plasma, beam, fibre, optics, camera, scanner and spectrometer parameters

Each of those sections controls appropriate aspect of simulation. For information on each parameter look at its description in configuration file.

A.3.7 Emission lines

List of emission lines suited for observations is placed in `<emission_parameters>` section:

```
<emission_lines description="CXRS elements to observe.">
    <HI>
        <name
            description="Name of the element."
            unit="n.a."
            type="str"
            value="hydrogen"/>
        <charge
            description="Charge of the ion."
            unit="n.a."
            type="int"
            value="0"/>
        <transition_levels
            description="Transition levels [upper, lower]."
            unit="n.a."
            type="int"
            value="[3, 2]"/>
    </HI>
    ... more lines omitted
</emission_lines>
```

You can change and add new entries in this section following given template. Added emission lines will be simulated if atomic data exists for them.

A.3.8 DNB

DNB section of the configuration file contains parameters for Diagnostic Neutral Beam. Structure of this section replicates structure of nbi IDS.

A.3.9 Wavelength ranges and geometry

These two sections contain all information for CXRS diagnostics.

B For Developers

B.1 Project Structure

Most of the functions implemented in this project contain docstrings written in "classic" Python style using **reStructuredText** syntax. Each docstring contains a short description of a function, list of arguments and their types and list of exceptions which can be risen during execution of the function.

B.2 Reading data from IMAS

Module responsible for reading data from IMAS and creating appropriate plasma and DNB models is stored in `cxrs/imas` directory.

B.2.1 Supplementary Functions

`ids_get` File `ids.py` contains only one function `ids_get` which is used to check and load requested IDS. For example

```
charge_exchange_ids = ids_get(
    name="charge_exchange",
    shot=134000,
    run=30,
    user="public",
    database="iter",
    version="3",
    occurrence=0
)
```

`name` is a name of requested IDS,
`shot` is an IMAS database shot ID,
`run` is an IMAS data run ID,
`user` is an IMAS database user ID,
`database` is an IMAS database ID,
`version` is an IMAS major version number,
`occurrence` is an IDS occurrence number. Each IDS can store several `occurrences` (refer to the description of an IDS). For example in `charge_exchange` IDS occurrences used to store data related to different diagnostics.

`find_nearest` File `find_nearest.py` contains only one function `find_nearest`. It is used for locating an index of the nearest time slice to the time requested by user.

Example:

```
idx = find_nearest(
    array=time_slices,
    value=260,
)
```

`array` is an input array,
`value` is a value to search for.

B.2.2 `equilibrium` IDS

File `equilibrium.py` contains `EquilibriumIDS` class which is used to read data from `equilibrium` IDS and create CHERAB's `EFITEquilibrium` object via `time` method. It is later used to build core plasma model.

Load an `equilibrium` IDS:

```
equilibrium_ids = EquilibriumIDS(
    shot=134000,
    run=30,
    user="public",
    database="iter",
    version="3",
)
```

`shot` is an IMAS database shot ID,
`run` is an IMAS data run ID,
`user` is an IMAS database user ID,
`database` is an IMAS database ID,
`version` is an IMAS major version number,

Create an `EFITEquilibrium` object:

```
equilibrium = equilibrium.time(time=-1)
```

`time` is a requested time. Here `-1` for time is used to acquire a time slice in the middle of time range.

Other methods:

`ids()` returns the `equilibrium` IDS object;
`psi_1d()` returns one-dimensional Ψ profile stored in `ids.time_slice[i].profiles_1d.psi`. It is implemented in case if `core_profiles` (section B.2.3) IDS does not contain its own profile.

B.2.3 `core_profiles` IDS

File `core_profiles.py` contains `CoreProfilesIDS` class which is used to read data from `core_profiles` IDS and create CHERAB's `Plasma` object via `create_plasma` method. It is poses as core plasma model.

Load a `core_profiles` IDS:

```
core_profiles_ids = CoreProfilesIDS(
    shot=134000,
    run=30,
    user="public",
```

```
        database="iter",
        version="3",
    )
```

`shot` is an IMAS database shot ID,
`run` is an IMAS data run ID,
`user` is an IMAS database user ID,
`database` is an IMAS database ID,
`version` is an IMAS major version number,

Create a `Plasma` object:

```
    core_plasma = core_profiles_ids.create_plasma(
        equilibrium=equilibrium,
        psi_1d=equilibrium.psi_1d(),
        integration_step=0.001,
        integration_samples=5,
        parent=world,
        transform=None,
        name="Core Plasma"
    )
```

`equilibrium` is an EFITEquilibrium object (section B.2.2);
`psi_1d` is one-dimensional Ψ profile (section B.2.2). It is used if one stored in `core_profiles` IDS is missing;
`integration_step` is step of volumetric integration in meters;
`integration_samples` is a number of integration samples;
`parent` is a parent node;
`transform` is transformation matrix;
`name` is a name of this plasma.
Note: for more information on `integration_step` and `integration_samples` refer to CHERAB's documentation on `Plasma`. For more information on `parent`, `transform` and `name` refer to Raysect's documentation on `Node`.

Note that `create_plasma` method does not require time value since it uses one that stored in `equilibrium`.

One required argument of `create_plasma` is `equilibrium`. It provides Ψ_{norm} distribution which is used to map density, temperature and bulk velocity distributions of plasma. Functions `distribution_density`, `distribution_temperature` and `distribution_velocity` are doing exactly that. *Note:* `distribution_temperature` tries to use average ion temperature or electron temperature if species' own temperature profile is absent in the IDS.

`detect_species` Function `detect_species` is used to recognize ion and neutral species from label given in IDS. Since there was no convention on the labeling at the time this appeared to be a huge problem. `detect_species` uses regular expressions to math species label along some other tricks. It returns CHERAB's `Element` object and species charge as a number (0 for neutrals).

```
species, charge = detect_species(
    structure=core_profiles_ids.ids.profiles_1d[0].ion[0],
    ion=True
)
```

`structure` is an IDS structure containing information on species (`ids.profiles_1d[i].ion[j]` or `ids.profiles_1d[i].neutral[j]`).

`ion` set to `True` for ion species or to `False` for neutrals. It changes regular expression pattern and sets `charge` to 0 for neutrals.

`distribution_density`

```
n_d = distribution_density(
    structure=core_profiles_ids.ids.profiles_1d[0].ion[0],
    symbol="D",
    charge=1,
    psi_normalised=psi_normalised,
    equilibrium=equilibrium
)
```

`structure` is an IDS structure containing information on species (`ids.profiles_1d[i].ion[j]` or `ids.profiles_1d[i].neutral[j]`).

`symbol` is a species symbol. It is used for messages.

`charge` is a species charge. It is used for messages.

`psi_normalised` is a Ψ_{norm} profile. It is used to map density values.

`equilibrium` is an EFITEquilibrium object (section B.2.2).

This function checks if density profile stored in the IDS is correct: not empty, greater than zero, not equal to zero and not equal to 1.0. If it is not correct than message is produced and this species is not included in the plasma model.

B.2.4 `edge_profiles` IDS

File `edge_profiles.py` contains `EdgeProfilesIDS` class which is used to read data from `edge_profiles` IDS and create CHERAB's `Plasma` object via `create_plasma` method. It is poses as edge plasma model.

`edge_profiles` IDS requires its own class because values there set to a mesh instead of 1D profile as in `core_profiles` IDS. Second reason is that

```
edge_profiles_ids = EdgeProfilesIDS(134000, 30)
edge_plasma = edge_profiles_ids.create_plasma(time=-1, parent=world)
# or
edge_plasma = edge_profiles_ids.create_plasma(equilibrium=equilibrium, parent=world)
```

B.2.5 `charge_exchange` IDS

File `charge_exchange.py` contains `ChargeExchangeIDS` class which is used to read data from `charge_exchange` IDS and create different types of observers.

```
charge_exchange_ids = ChargeExchangeIDS(134000, 30)
sightlines = SightlineGroup(ids=charge_exchange_ids, parent=world)
```

B.2.6 `nbi` IDS

File `nbi.py` contains `NBIIDS` class which is used to read data from `nbi` IDS and create CHERAB's `Beam` object via `create_beam` method. It is poses as DNB model.

```
nbi_ids = NBIIDS(134000, 30)
beam = nbi_ids.create_beam(
    time=-1,
    plasma=core_plasma,
    atomic_data=adas,
    attenuation_instructions=attenuation_instructions,
    emission_instructions=emission_instructions,
    parent=world
)
```

At the time `Beam` supports model with only one beamlet and `create_beam` is designed with this in mind.

B.3 Setting the Wall

File `cxrs/machine/pfc_mesh.py` contains function `load_pfc_mesh` that is used to create a reactor wall model. All meshes are stored in `machine/portplugs` and `machine/simple` subfolders.

```
wall = load_pfc_mesh(
    reflections=True,
    roughness={"Be": 0.26, "W": 0.29, "Ss": 0.13}
    parent=world,
)
```

where `reflections` assigns material properties to appropriate wall segments if set to `True` and sets the wall as perfect absorber if set to `False`. It is used to effectively turn reflections on and off. `roughness` argument sets *roughness* of the materials assigned to the wall segments (beryllium, tungsten and stainless steel).

B.4 Observers

Module `cxrs/observers` contains several files defining different observer classes built upon Raysect's observers.

B.4.1 Base Class

File `observers/base` contains `ObserverGroup` class that represents a group of observers, for example CXRS sightlines. The class has `observe` method that is used to perform an observation by all observers in a group one by one and store the results. Methods `display` and `savetxt` are used to show registered spectra as an image or plot and save results in the text format respectively. They should be implemented in subclasses.

Example:

```
ObserverGroup(
    charge_exchange_ids=charge_exchange_ids,
    config="config.xml",
    wavelength_range=1,
    relative_error=0.05,
    scenario=scenario,
    parent=world,
    transform=None,
    name="CXRS Edge Sightlines"
)
```

`charge_exchange_ids` is a `ChargeExchangeIDS` object (section B.2.5),
`config` is a path to configuration file,
`wavelength_range` is a number representing a wavelength range for observation (it is defined in a configuration file),
`relative_error` is a minimal value of a desired relative error (if achieved relative error is higher than this value, number of pixel samples will be increased and observation will be performed again until desired relative error is achieved),
`scenario` is a dictionary containing all simulation labels: shot number, run number, time, used emission types, etc.,
`parent` is a parent node in a scenegraph,
`transform` is a transformation matrix,

`name` is a name for this group of observers.

B.4.2 Sightlines

B.4.3 Optics

B.4.4 Fibres

B.4.5 Camera

B.4.6 Others

B.5 Populating CHERAB's Atomic Database

B.6 Utility Functions

B.6.1 Parsing XML Configuration File

B.6.2 Setting Emission Parameters

B.6.3 Math Functions

B.6.4 Others