giwaxs_forward_sim

Instruction Manual

Requirements:

- python 3
- numpy
- matplotlib
- fabio
- scipy

Usage:

Forward simulations are created through two different scripts: *generate_iq_voxelgrid.py* and *generate_detector_images.py*. These scripts are intended to be ran in the command line with a single argument pointing to the configuration file.
(ex: `python generate_iq_voxelgrid.py ––config /path/to/config_file.txt`).
Details of these scripts and their configuration file formats are described below:

***generate_iq_voxelgrid.py*:**

This script takes a .xyz file and converts it into a 3D voxel grid of scattering intensity values with axes in units of Å^{-1} through the following steps:
1. Mapping the .xyz file onto an electron density voxel grid.
2. Taking the FFT of the electron density voxel grid
3. taking amplitude of values, recentering axes, converting to q-units, and applying a general atomic form factor.
4. Cropping reciprocal space voxel grid to relevant q-values and saving them for later use

Configuration file parameters:
An example configuration file is in */config_templates/ iq_voxelgrid_config.txt*
xyz_path – (string) path to a .xyz file you would like to generate I vs q voxel grid for
gen_name – (string) a short sample name used to create directories and output files
voxel_size – (positive float) side length dimension of square real-space voxels in Å
min_ax_size – (positive integer) minimum number of voxels along each axis
f0_element – (string) elemental symbol for z-normalized f0(q) scaling
max_q – (positive float) determines the q-value which the iq voxel grid is cropped to
output_dir – (string) path to output directory, if not defined os.get_cwd() is used

Tips:

- It is advantageous to choose axis length that is larger than the slab described by the .xyz file. This “padding” can lower the bin size of the FFT resulting in better q-resolution
- For computation speed, min_ax_length should ideally be a power of 2. Avoid primes
- Carefully choose the real-space voxel dimension since it will carry over as q-uncertainty
- The slabs described by the .xyz file should be orthorhombic to allow for the code to properly padding with an average electron density to best prevent termination ripples in the reciprocal space.

***generate_detector_images.py*:**
This script loads the iq reciprocal space voxel grid and associated axes that were generated by *generate_iq_voxelgrid.py* and uses them to populate scattering intensity on a 2D detector plane at various geometries. These geometries are summed to produce a final "det_sum" as the simulated GIWAXS. The steps for completing this are:
1. Initializing detector plane size, resolution, and orientation
2. Intersecting detector pixels with scattering intensity voxels
3. Saving detector intensities at that orientation
4. Rotating detector and repeating step 3 for all orientations
4. Summing final detector image of all orientations

Configuration file parameters:
An example configuration file is in */config_templates/ detector_image_config.txt*
iq_output_folder-(string) output from *generate_iq_voxelgrid.py* (form '*name_output_files/*')
gen_name-(string) same gen_name used in *generate_iq_voxelgrid.py*
max_q-(positive float) maximum q-value on detector, must be <=max_q used to make iq file
num_pixels-(positive integer) number of pixels along each detector axis
angle_init_val1-(float) 1st initializing detector rotation in degrees about angle_init_ax1
angle_init_val2-(float) 2nd initializing detector rotation in degrees about angle_init_ax2
angle_init_val3-(float) 3rd initializing detector rotation in degrees about angle_init_ax3
angle_init_ax1-(string) rotation axis for 1st initializing rotation, set to none for no rotation
angle_init_ax2-(string) rotation axis for 2nd initializing rotation, set to none for no rotation
angle_init_ax3-(string) rotation axis for 3rd initializing rotation, set to none for no rotation
psi_start-(float) starting value in degrees for psi
psi_end-(float) ending value in degrees for psi
psi_num-(positive integer) number of linearly spaced psi steps
phi_start-(float) starting value in degrees for phi
phi_end-(float) ending value in degrees for phi
phi_num-(positive integer) number of linearly spaced phi steps

Tips:
- Rotation axes are defined as psi, phi, and theta for rotation about detector normal, vertical, and horizontal axes respectively
- The detector begins with vertical axis pointing along positive qz, horizontal axis along positive qy, and normal axis along positive qx
- Use "init" rotations to set up your detector such that psi and phi will capture the disorder you desire. Phi is usually used for fiber texture and psi for orientational disorder
- Visualization tools are available as jupyter notebooks in ./test_notebooks to better understand these manipulations
- Only ¼ of the total rotation space needs to be probed as the GIWAXS detector plane is mirrored about horizontal and vertical axis after summing
- For example, if you are trying to match an experimental sample with fiber texture and ±15° tilting about the backbone axis then you may define psi_start, end, num=(0,15,16) and phi_start, end, num=(0,179, 180).

Other tools:

xyz_slab_generator.py
This script takes an .xyz periodic unit cell and propogates it to a desired orthorhombic slab size.

Configuration file parameters:
An example configuration file is in */config_templates/ xyz_slab_config.txt*
input_filepath-(string) path to .xyz cell (ex: ./test_xyz_files/graphite_UnitCell.xyz)
output_filepath-(string) directory where you would like .xyz slab saved (optional)
gen_name-(string) same gen_name used in *generate_iq_voxelgrid.py*
x_size-(float) size in Å of slab along x-axis
y_size -(float) size in Å of slab along y-axis
z_size-(float) size in Å of slab along z-axis
a=(float) cell side length Å
b=(float) cell side length Å
c=(float) cell side length Å
alpha-(float) cell interior angle degrees
beta-(float) cell interior angle degrees
gamma-(float) cell interior angle degrees

plotting_and_comparing.py
Script in progress. Current tools are contained in jupyter notebooks in test_notebooks folder