

BornAgain - simulating and fitting X-ray and neutron
small angle scattering at grazing incidence.

User Guide

version 0.1

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Introduction

BornAgain is a software to simulate and fit small-angle scattering at grazing incidence (GISAS). It support analysis both X-ray (GISAXS) and neutron (GISANS) data. The name of the software, BornAgain, indicates the central role of the distorted-wave Born approximation (DWBA) in the physical description of the scattering process. The software provides a generic framework for modeling multilayer samples with smooth or rough interfaces and with various types of embedded nanoparticles. In this way, it reproduces and enhances the functionality of the present reference software, IsGISAXS by R. Lazzari [?], and lays a solid base for future extensions in response to specific user needs.

To meet the growing demand for GISAS simulation of more complex structured materials, BornAgain has extended the IsGISAXS program's functionality by removing the restrictions on the number of layers and particles, by providing diffuse reflection from rough layer interfaces and by adding particles with inner structure.

BornAgain is platform independent software, with active support for Linux, MacOS and Microsoft Windows (planned for October, 2013). It is free and open source software provided under terms of GNU General Public License (GPL). The authors will be grateful for all kind of feedback: criticism, praise, bug reports, feature requests, contributed modules. When BornAgain is used in preparing scientific papers, please cite this manual as follows:

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BornAgain - simulating and fitting X-ray and neutron small angle scattering at grazing incidence,
<http://apps.jcns.fz-juelich.de/BornAgain>

This user guide starts with a brief description of the steps necessary for compiling the source code and running the simulation in Section 1.1. More detailed overview of software architecture and installation procedure are given in Section 1.2 and Section 1.3. General methodology of simulation with BornAgain and detailed usage examples are given in Section ???. Fitting tools provided by the framework are presented in Section ???.

Icons used in this manual:



: this sign highlights further references.



: this sign highlights essential points.

Chapter 1

Installation

1.1 Quick start

This section shortly describes how to build BornAgain from source and run the first simulation. More details about software architecture and installation procedure are given in Section 1.2 and Section 1.3.

Step I: installing third party software

- compilers: clang versions ≥ 3.1 or GCC versions ≥ 4.2
- cmake (≥ 2.8)
- boost library (≥ 1.48)
- GNU scientific library (≥ 1.15)
- fftw3 library ($\geq 3.3.1$)
- python-2.7, python-devel, python-numpy-devel

Step II: getting the source

```
git clone git://apps.jcns.fz-juelich.de/BornAgain.git
```

Step III: building the source

```
mkdir <build_dir>; cd <build_dir>;  
cmake <source_dir> -DCMAKE_INSTALL_PREFIX=<install_dir>  
make  
make check  
make install
```

Step IV: running example

```
cd <install_dir>/Examples/python/ex001_CylindersAndPrisms  
python CylindersAndPrisms.py
```

1.2 Software architecture

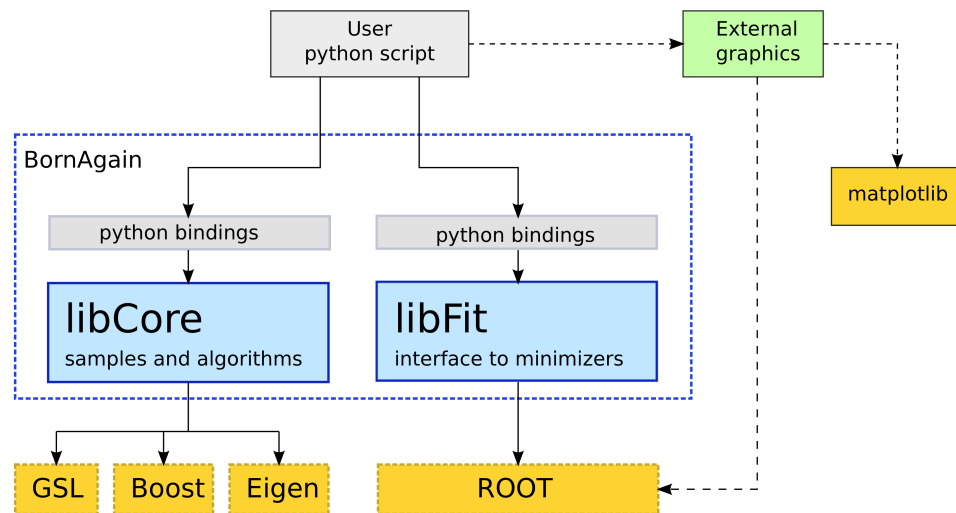


Figure 1.1: Structure of BornAgain libraries.

1.3 Installation

This section describes how to build and install BornAgain libraries from the source. At the moment we support building on x86/x86_64 Linux and Mac OS X operating systems. Support for Windows systems is planned in next releases. There are three major steps to building BornAgain :

1. Acquire required third-party libraries.
2. Get BornAgain source code.
3. Use cmake to build and install software.

The remainder of this section explains each step in detail.

1.3.1 Third-party software.

To successfully build BornAgain a number of prerequisite packages must be installed.

- compilers: clang versions ≥ 3.1 or GCC versions ≥ 4.2
- cmake (≥ 2.8)
- boost library (≥ 1.48)
- GNU scientific library (≥ 1.15)
- fftw3 library (≥ 3.3)
- python (≥ 2.7 , < 3.0), python-devel, python-numpy-devel

Other packages are optional

- ROOT framework (adds several additional fitting algorithms to BornAgain)
- python-matplotlib (allows to run usage examples with graphics)

All required packages can be easily installed on most Linux distributions using the system's package manager. Below we give a few examples for several selected operation systems. Please note, that other distributions (Fedora, Mint, etc) may have different commands for invoking the package manager and slightly different names of packages (like “boost” instead of “libboost” etc). Besides that, the installation should be very similar.

OpenSuse 12.3

Adding “scientific” repository

```
sudo zypper ar http://download.opensuse.org/repositories/science/
openSUSE_12.3 science
```

Installing required packages

```
sudo zypper install git-core cmake gsl-devel boost-devel fftw3-devel
python-devel python-numpy-devel
```

Installing optional packages

```
sudo zypper install libroot-* root-plugin-* root-system-* root-ttf
libeigen3-devel python-matplotlib
```

Ubuntu 12.10, 13.04

Installing required packages

```
sudo apt-get install git cmake libgsl0-dev libboost-all-dev libfftw3-dev  
python-dev python-numpy
```

Installing optional packages

```
sudo apt-get install libroot-* root-plugin-* root-system-* ttf-root-  
installer libeigen3-dev python-matplotlib python-matplotlib-tk
```

Mac OS X 10.8

To simplify the installation of third party open-source software on a Mac OS X system we recommend the use of MacPorts package manager. The easiest way to install MacPorts is by downloading the dmg from www.macports.org/install.php and running the system's installer. After the installation new command “port” will be available in terminal window of your Mac.

Installing required packages

```
sudo port -v selfupdate  
sudo port install git-core cmake  
sudo port install fftw-3 gsl  
sudo port install boost -no_single -no_static+python27
```

Installing optional packages

```
sudo port install py27-matplotlib py27-numpy py27-scipy  
sudo port install root +fftw3+python27  
sudo port install eigen3
```

1.3.2 Getting source code

BornAgain source can be downloaded at <http://apps.jcns.fz-juelich.de/BornAgain> and unpacked with

```
tar xzf bornagain-<version>.tgz
```

Alternatively one can obtain BornAgain source from our public Git repository.

```
git clone git://apps.jcns.fz-juelich.de/BornAgain.git
```

More about Git

Our Git repository holds two main branches called “master” and “develop”. We consider “master” branch to be the main branch where the source code of HEAD always reflects latest stable release. git clone command shown above

1. gives you a source code snapshot corresponding to the latest stable release,
2. automatically sets up your local master branch to track our remote master branch, so you will be able to fetch changes from the remote branch at any time using “git pull” command.

Master branch is updating approximately once per month. The second branch, “develop” branch, is a snapshot of the current development. This is where any automatic nightly builds are built from. The develop branch is always expected to work, so to get the most recent features one can switch source code to it by

```
cd BornAgain
git checkout develop
git pull
```

1.3.3 Building and installing the code

BornAgain should be build using CMake cross platform build system. Having third-party libraries installed on the system and BornAgain source code acquired as was explained in previous sections, type build commands

```
mkdir <build_dir>
cd <build_dir>
cmake <source_dir> -DCMAKE_INSTALL_PREFIX=<install_dir>
make
```

Here <source_dir> is the name of directory, where BornAgain source code has been copied, <install_dir> is the directory, where user wants the package to be installed, and <build_dir> is the directory where building will occur.

About CMake



Having dedicated directory <build_dir> for build process is recommended by CMake. That allows several builds with different compilers/options from the same source and keeps source directory clean from build remnants.

Compilation process invoked by the command “make” lasts about 10 min for an average laptop of 2012 edition. On multi-core machines the compilation time can be decreased by invoking command “make” with the parameter “make -j[N]”, where N is the number of cores.

Running functional tests is an optional but recommended step. Command “make check” will compile several additional tests and run them one by one. Every test contains the simulation of a typical GISAS geometry and the comparison on numerical level of simulation results with reference files. Having 100% tests passed ensures that your local installation is correct.

```
make check
...
100% tests passed, 0 tests failed out of 26
Total Test time (real) = 89.19 sec
[100%] Build target check
```

The last command “make install” copies compiled libraries and some usage examples into the installation directory.

```
make install
```

Troubleshooting

In the case of complex system setup, with variety of libraries of different versions scattered across multiple places (/opt/local, /usr etc.), you may want to help CMake to find libraries in proper place. In example below two system variables are defined to force CMake to prefer libraries found in /opt/local to other places.


```
export CMAKE_LIBRARY_PATH=/opt/local/lib:$CMAKE_LIBRARY_PATH
export CMAKE_INCLUDE_PATH=/opt/local/include:$CMAKE_INCLUDE_PATH
```

If compilation fails for some reason, please submit your bug report including compilation errors at <http://apps.jcns.fz-juelich.de/redmine/projects/bornagain/issues>

1.3.4 What is next?

In your installation directory you will find

```
./include - header files for compilation of your C++ program
./lib - libraries to import into python or link with your C++ program
./Examples - directory with examples
```

Run your first example and enjoy first BornAgain simulation plot.

```
cd <install_dir>/Examples/python/ex001_CylindersAndPrisms
python CylindersAndPrisms.py
```

Chapter 2

Examples

2.1 General methodology

A simulation of GISAXS using BornAgain platform can be decomposed into the following points:

- Definition of the materials by specifying their names and their refractive indices,
- Definition of particles: shapes, sizes, refractive indices of the constituting material, interference functions,
- Definition of the layers: thicknesses, roughnesses, associations with the previously defined materials,
- Inclusion of the particles in layers: **density or proportion**, positions, orientations,
- Assembling the sample: generation of a multilayered system,
- Specifying the input beam and the output detector's characteristics,
- Running the simulation,
- Saving the data.

The sample is built from object oriented building blocks instead of loading data files.

2.2 Conventions

2.2.1 Geometry of the sample

The geometry used to describe the sample is shown in Fig. 2.1. The z -axis is perpendicular to the sample's surface and pointing upwards. The x -axis is perpendicular to the plane of the detector and the y -axis is along it. The input and the scattered output beams are each by two angles α_0, ϕ_0 and α_f, ϕ_f respectively. Then for each other layer $j = 1, \dots, N - 1$, the incident angles α_j and ϕ_j are defined with respect to the bottom of the layer. Our choice of orientation for the angles α_j is so that α_0 and α_f shown in fig. 2.1 are positive.

The layers are defined by their thicknesses (parallel to the z -direction), their possible roughnesses (equal to 0 by default) and the refractive index of the material. We do not define any dimensions

in the x, y directions. And, except for roughness, the layer's vertical boundaries are plane and perpendicular to the z -axis. There is also no limitation to the number of layers that could be defined in BornAgain.



Remark - Order of the different steps for the simulation:

When assembling the sample, the layers are defined from top to bottom. So in most cases the first layer will be the air layer.

The particles are characterized by their form factors (*i.e.* the Fourier transform of the shape function - see the list of form factors implemented in BornAgain) and the refractive index of the composing material. The number of input parameters for the form factor depends on the particle symmetry; it ranges from one parameter for a sphere (its radius) to three for an ellipsoid (its three main axis lengths).

By placing the particles inside or on top of a layer, we impose their vertical positions. The in-plane distribution of particles is linked with the way the particles interfere with each other, which is therefore implemented when dealing with the interference function.



Remark - Depth of particles

The vertical positions of particles in a layer are given in relative coordinates. For the top layer, the bottom corresponds to $\text{depth}=0$. But for all the other layers, it is the top of the layer which corresponds to $\text{depth}=0$.

The complex refractive index associated with a layer or a particle is written as $n = 1 - \delta + i\beta$, with $\delta, \beta \in \mathbb{R}$. In our program we input δ and β directly.

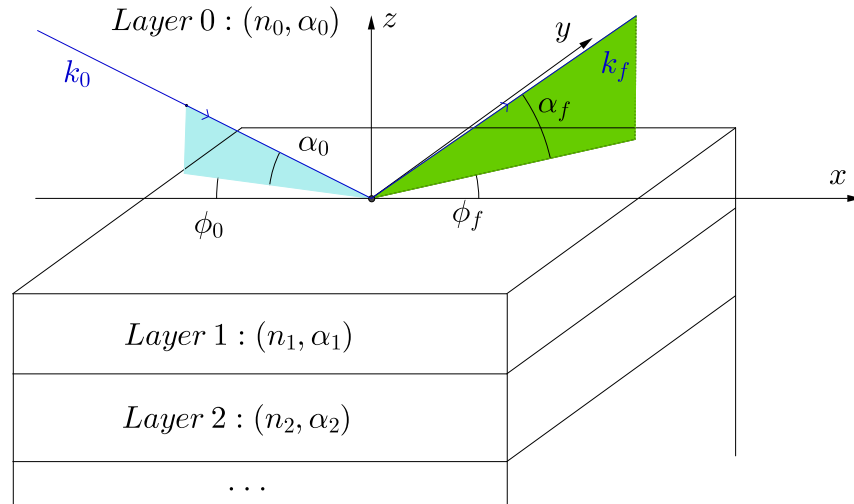


Figure 2.1: Representation of the scattering geometry for multilayer specular reflectivity. n_j is the refractive index of layer j and α_j is the incident angle of the wave propagating in layer j and incident on layer $j + 1$. α_f is the exit angle with respect to the sample's surface and ϕ_f is the scattering angle with respect to the scattering plane.

The input beam is assumed to be monochromatic without any spatial divergence.

polarization term?

2.2.2 Units

By default angles are expressed in radians and lengths are given in nanometers. But it is possible to use other units by specifying them right after the value of the corresponding parameter like, for example, `20.0*Units::micrometer` in C++.

2.2.3 Programs



Programming The examples presented in the next paragraphs are written in C++ or Python. For tutorials about these programming languages, the users are referred to [?] and [?] respectively.

Note about the version of C++ and Python to run the examples.

Where can the following examples be found?

What is the command to run the examples?

2.3 Example 1: Two types of islands on top of substrate. No interference function

In this example, using Python language, we simulate the scattering from a mixture of cylindrical and prismatic nanoparticles without any interference between them. These particles are placed in air, on top of a substrate.

We are going to go through each step of the simulation. The Python script specific to each stage will be given at the beginning of the description. But for the sake of completeness the full code is given at the end of this section (Listing 2.1).

We start by importing different functions from external modules (lines 1-7). For example, line 3 imports NumPy, which is a fundamental package for scientific computing with Python (<http://www.numpy.org/>). In particular, line 7 imports the features of BornAgain software.

Finally line 9 marks the beginning of the function to define and run the simulation.

```

1  import sys
2  import os
3  import numpy
4
5  sys.path.append(os.path.abspath(os.path.join(os.path.split(__file__)[0],
        '..', '..', '..', 'lib')))
6
7  from libBornAgainCore import *
8
9  def RunSimulation():

```

First step: Defining materials

```

10 # defining materials
11 mAmbience = MaterialManager.getHomogeneousMaterial("Air", 0.0, 0.0 )

```

```
12 mSubstrate = MaterialManager.getHomogeneousMaterial("Substrate", 6e-6, 2
    e-8)
```

Lines 11 and 12 define two different materials using function `getHomogeneousMaterial` from class `MaterialManager`. The general syntax is the following

```
Interface material name = MaterialManager.getHomogeneousMaterial("name",
    delta, beta)
```

where `name` is the name of the material associated with its complex refractive index $n=1-\delta + i\beta$. Interface `material name` is later used when referring to this particular material. The two defined materials in this example are Air with a refractive index of 1 ($\delta = \beta = 0$) and a Substrate associated with a complex refractive index equal to $1 - 6 \times 10^{-6} + i2 \times 10^{-8}$.

Remark: there is no condition on the choice of name.

Second step: Defining the particles

```
13 # collection of particles
14 n_particle = complex(6e-4, 2e-8)
15 cylinder_ff = FormFactorCylinder(5*nanometer, 5*nanometer)
16 cylinder = Particle(n_particle, cylinder_ff)
17 prism_ff = FormFactorPrism3(5*nanometer, 5*nanometer)
18 prism = Particle(n_particle, prism_ff)
```

We implement two different shapes of particles: cylinders and prisms (*i.e.* elongated particles with a constant equilateral triangular cross section).

All particles implemented in `BornAgain` are defined by their form factors, their sizes and the refractive index of the material they are made of. Here, for the cylindrical particle, we input its radius and its height. For the prism, the possible inputs are the length of one side of its equilateral triangular base and its height.

In line 14, we define the complex refractive index associated with both particle shapes: $n=1 - 6 \times 10^{-4} + i2 \times 10^{-8}$.

In order to define a particle, we proceed in two steps. For example for the cylindrical particle, we first specify the form factor of a cylinder with its radius and height, both equal to 5 nanometers in this particular case (see line 15). Then we associate this shape with the refractive index of the constituting material as in line 16.

The same procedure has been applied for the prism in lines 17 and 18 respectively.

Third step: Characterizing the layers and assembling the sample

Particle decoration

```
19 particle_decoration = ParticleDecoration()
20 particle_decoration.addParticle(cylinder, 0.0, 0.5)
21 particle_decoration.addParticle(prism, 0.0, 0.5)
22 interference = InterferenceFunctionNone()
23 particle_decoration.addInterferenceFunction(interference)
```

The process of defining the positions and densities of particles in our sample is called “particle decoration”. We use the function `ParticleDecoration()` (line 19) and the associated `addParticle` for each particle shape (lines 20, 21). The general syntax is

```
particledcoration.addParticle(particle_name , depth , abundance)
```

where `particle_name` is the name used to define the particles (lines 16 and 18), `depth` (default value =0) is the vertical position, expressed in nanometers, of the particles in a given layer (the association with a particular layer will be done during the next step) and `abundance` is the proportion of this type of particles, normalized to the total number of particles. Here we have 50% of cylinders and 50% of prisms.

Remark - Depth of particles



The vertical positions of particles in a layer are given in relative coordinates. For the top layer, the bottom corresponds to `depth=0` and negative values would correspond to particles floating above layer 1 since the vertical axis, shown in fig. 2.1 is pointing upwards. But for all the other layers, it is the top of the layer which corresponds to `depth=0`.

Finally lines 22 and 23 specify that there is **no coherent interference** between the waves scattered by these particles. The intensity is calculated by the incoherent sum of the scattered waves: $\langle |F_n|^2 \rangle$, where F_n is the form factor associated with the particle of type n . The way these waves interfere imposes the horizontal distribution of the particles as the interference reflects the long or short-range order of the particles distribution (**see Theory**). On the contrary, the vertical position is imposed when we add the particles in a given layer by parameter `depth`, as shown in lines 20 and 21.

Multilayer

```
24 # air layer with particles and substrate form multi layer
25 air_layer = Layer(mAmbience)
26 air_layer_decorator = LayerDecorator(air_layer , particle_decoration)
27 substrate_layer = Layer(mSubstrate , 0)
28 multi_layer = MultiLayer()
29 multi_layer.addLayer(air_layer_decorator)
30 multi_layer.addLayer(substrate_layer)
```

We now have to configure our sample. For this first example, the particles, *i.e.* cylinders and prisms, are on top of a substrate in an air layer. **The order in which we define these layers is important: we start from the top layer down to the bottom one.**

Let us start with the air layer. It contains the particles. In line 25, we use the previously defined `mAmbience` (=“air” material) (line 11). The command written in line 26 shows that this layer is decorated by adding the particles using the function `particledcoration` defined in lines 19-23. Note that the `depth` is referenced to the bottom of the top layer (negative values would correspond to particles floating above layer 1 as the vertical axis is pointing upwards). The substrate layer only contains the substrate material (line 27).

There are different possible syntaxes to define a layer. As shown in lines 25 and 27, we can use `Layer(Interface material name,thickness)` or `Layer(Interface material name)`. The second case corresponds to the default value of the thickness, equal to 0. The thickness is expressed in nanometers.

Our two layers are now fully characterized. The sample is assembled using `MultiLayer()` constructor (line 28): we start with the air layer decorated with the particles (line 29), which is the layer at the top and end with the bottom layer, which is the substrate (line 30).

Fourth step: Characterizing the input beam and output detector and running the simulation

```

31 # run simulation
32 simulation = Simulation()
33 simulation.setDetectorParameters(100, -1.0*degree, 1.0*degree,
34                                100, 0.0*degree, 2.0*degree, True)
35 simulation.setBeamParameters(1.0*angstrom, 0.2*degree, 0.0*degree)
36 simulation.setSample(multi_layer)
37 simulation.runSimulation()

```

The first stage is to define the `Simulation()` object (line 32). Then we define the detector (line 34) and beam parameters (line 35), which are associated with the sample previously defined (line 36). Finally we run the simulation (line 37). Those functions are part of the `Simulation` class. The different incident and exit angles are shown in Fig. 2.1.

The detector parameters are set using ranges of angles via the function:

```

setDetectorParameters(n_phi, phi_f_min, phi_f_max,
                     n_alpha, alpha_f_min, alpha_f_max, isgisaxs_style=false),

```

where $n_phi=100$ is the number of points in the range of variations of angle ϕ_f , $phi_f_min=-1.0*degree$ and $phi_f_max=1.0*degree$ are the minimum and maximum values respectively of ϕ_f , which is the in-plane direction of the scattered beam (measured with respect to the x -axis), $n_alpha=100$ is the number of points in the range of variations of the exit angle α_f measured from the x, y -plane in the z -direction, $alpha_f_min=0.0*degree$ and $alpha_f_max=2.0*degree$ are the minimum and maximum values respectively of α_f , $isgisaxs_style=True$ (default value = False) is a boolean used to characterise the structure of the output data. If $isgisaxs_style=True$, the output data is binned at constant values of the sine of the output angles, α_f and ϕ_f , otherwise it is binned at constant values of these two angles.

For the beam the function to use is `simulation.setBeamParameters(lambda, alpha_i, phi_i)`, where $lambda=1.0*angstrom$ is the incident beam wavelength, $alpha_i=0.2*degree$ is the incident grazing angle on the surface of the sample, $phi_i=0.0*degree$ is the in-plane direction of the incident beam (measured with respect to the x -axis). Note that in Fig. 2.1 $\alpha_i = \alpha_0$ and $\phi_i = \phi_0$.

Remark: Note that, except for `isgisaxs_style`, there are no default values implemented for the parameters of the beam and detector.

Line 37 shows the command to run the simulation using the previously defined setup.

Fifth step: Saving the data

```

38 # retrieving intensity data
39 return GetOutputData(simulation) %arr = GetOutputData(simulation)

```

In line 39 we record the simulated intensity as a function of outgoing angles α_f and ϕ_f for further uses (plots, fits,...) as a NumPy array containing $n_phi \times n_alpha$ datapoints. Some options are provided by BornAgain. For example, figure 2.2 shows the two-dimensional contourplot of the intensity as a function of α_f and ϕ_f .

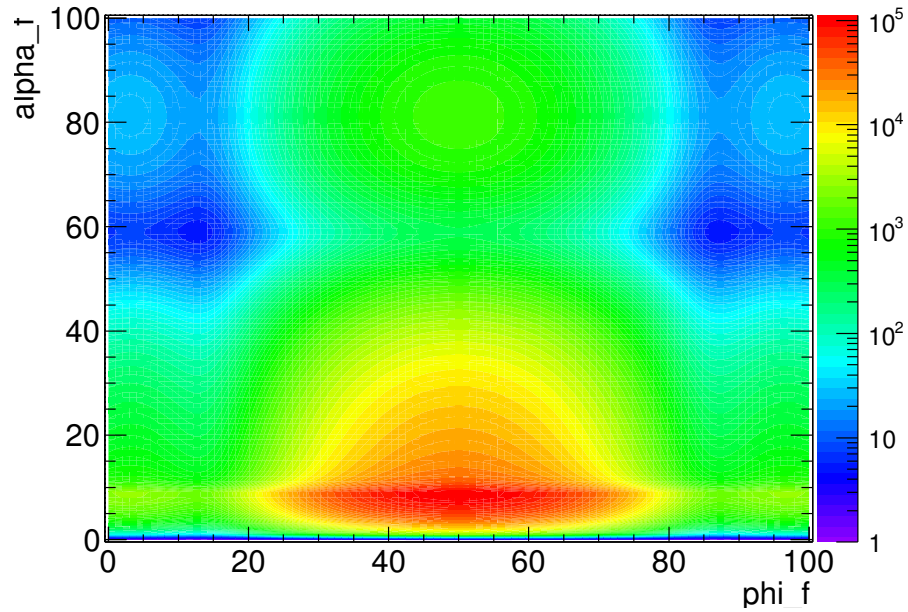


Figure 2.2: Figure of example 1: Simulated grazing-incidence small-angle X-ray scattering from a mixture of cylindrical and prismatic nanoparticles without any interference, deposited on top of a substrate. The input beam is characterized by a wavelength λ of 1 Å and incident angles $\alpha_i = 0.2^\circ$, $\phi_i = 0^\circ$. The cylinders have a radius and a height both equal to 5 nm, the prisms are characterized by a side length equal to 5 nm and they are also 5 nm high. The material of the particles has a refractive index of $1 - 6 \times 10^{-4} + i2 \times 10^{-8}$. For the substrate it is equal to $1 - 6 \times 10^{-6} + i2 \times 10^{-8}$. The colorscale is associated with the output intensity in arbitrary units.


```

import sys
import os
import numpy

sys.path.append(os.path.abspath(os.path.join(os.path.split(__file__)[0],
    '..', '..', '..', 'lib')))

from libBornAgainCore import *

def RunSimulation():
    # defining materials
    mAmbience = MaterialManager.getHomogeneousMaterial("Air", 0.0, 0.0 )
    mSubstrate = MaterialManager.getHomogeneousMaterial("Substrate", 6e
        -6, 2e-8)
    # collection of particles
    n_particle = complex(6e-4, 2e-8)
    cylinder_ff = FormFactorCylinder(5*nanometer, 5*nanometer)
    cylinder = Particle(n_particle, cylinder_ff)
    prism_ff = FormFactorPrism3(5*nanometer, 5*nanometer)
    prism = Particle(n_particle, prism_ff)
    particle_decoration = ParticleDecoration()
    particle_decoration.addParticle(cylinder, 0.0, 0.5)
    particle_decoration.addParticle(prism, 0.0, 0.5)
    interference = InterferenceFunctionNone()
    particle_decoration.addInterferenceFunction(interference)
    # air layer with particles and substrate form multi layer
    air_layer = Layer(mAmbience)
    air_layer_decorator = LayerDecorator(air_layer, particle_decoration)
    substrate_layer = Layer(mSubstrate, 0)
    multi_layer = MultiLayer()
    multi_layer.addLayer(air_layer_decorator)
    multi_layer.addLayer(substrate_layer)

    # run simulation
    simulation = Simulation()
    simulation.setDetectorParameters(100, -1.0*degree, 1.0*degree,
        100, 0.0*degree, 2.0*degree, True)
    simulation.setBeamParameters(1.0*angstrom, 0.2*degree, 0.0*degree)
    simulation.setSample(multi_layer)
    simulation.runSimulation()

    # retrieving intensity data
    return GetOutputData(simulation)

```

Listing 2.1: Python script of example 1

2.4 Example 2