Experiment planning, simulation and fitting of GISAS data using the BornAgain framework - recent developments and advanced applications.

M. Ganeva, J. Fisher[1], J.C. Loaiza, G. Pospelov, W. Van Herck, J. Wuttke and D. Yurov

Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ),

Forschungszentrum Jülich GmbH, Garching, Germany

[1]Cape Analytics GmbH, München, Germany

One of the main challenges for the successfull interpretation of feature rich data in the field of surface neutron and X-ray scattering rests with the accurate parametric data modelling and fitting. A community recognized software which gives access to the corresponding functionality in a reliable and user friendly manner, is of key importance for scientists running their experiments at various neutron and synchrotron facilities.

BornAgain [1] is a generic framework that provides scientists with the means for modelling multilayer samples with smooth or rough interfaces, various types of embedded nanoparticles and various models to treat finite size effects and the coupling between the type and position of a particle. Its name, BornAgain, alludes to the central role of the distorted-wave Born approximation in the physical description of the scattering process.

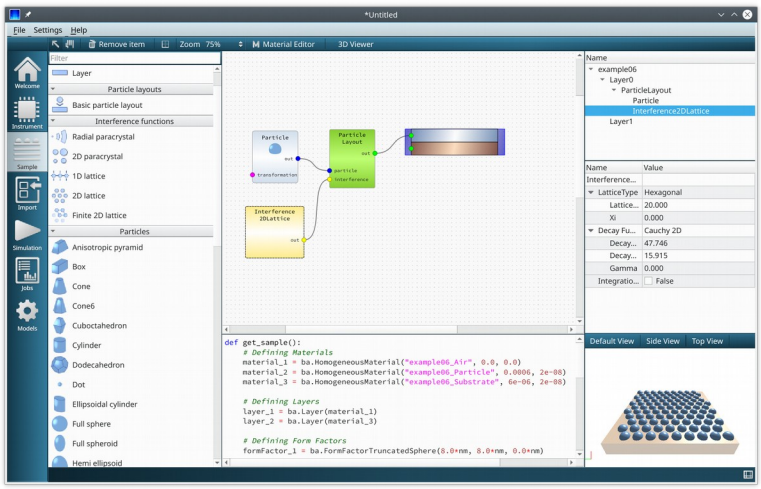

Figure 1: BornAgain graphical user interface

Carefully designed for a broad community of users, BornAgain offers a modern graphical user interface with the possibility to perform real-time simulations and to fit experimental data. The recent developments, such as a 3D real-space sample view and advanced instrument geometries facilitates virtual sample preparation and experiment planning.

BornAgain development has started in 2012 and initialy the project was oriented to the needs of the users from the grazing incidence community with the aim to supersede the highly successful but no longer actively developed software IsGisaxs [2]. Since that time the project was continuously evolving following the requests of the growing user community to support multilayer samples of various complexity: from well ordered nanoparticle arrays [3] to disordered soft matter systems [4]. Currently the software supports both nuclear and magnetic neutron scattering, offering the user a way to analyze polarized SANS and GISANS [5].

Lately we have started to extend BornAgain from GISAS to specular reflectometry and off-specular scattering with the idea to provide scientists with a universal tool to plan and analyse their specular, off-specular and GISAS experiments within a single framework.

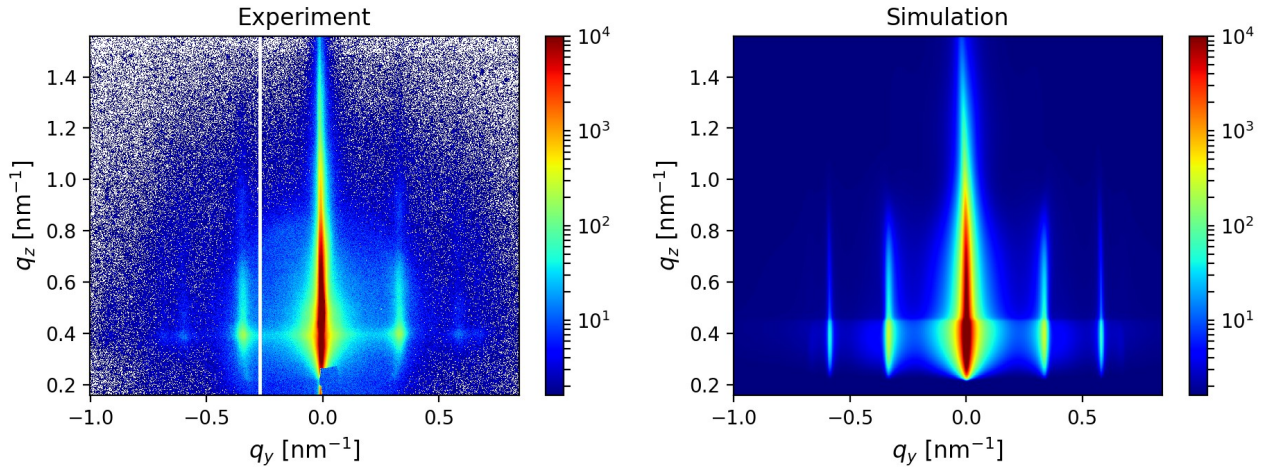

Figure 1: Close packed hexagonal monolayer, BornAgain/experiment comparison [3].

The BornAgain framework is fully exposed to Python to allow users to create complex sample models, define experimental geometries and fully control the analysis workflow. Particularly, it makes possible to go beyond conventional data fitting and to meet the challenge of automatic data analysis by using deep neural networks. Here, the role of BornAgain as an efficient platform for generating training data is self-evident.

The framework is actively maintained, free, open-source and released under the GPL3 license. It is multi platform, adherent to object-oriented design, fosters a professional approach to software development and lays a solid foundation for future extensions in response to specific user needs.

References

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