# BornAgain: simulating X–ray and neutron scattering at grazing incidence

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Owing to the wealth of information contained in the detector image of grazing incidence small angle scattering experiments (GISAS), these are increasingly used to investigate the structural properties of thin films, layered materials, nanoparticle depositions and many others. Due to this very same nature however, the technique is quite computation–intensive and a scientifically sound interpretation of the scattering data requires comparison with numerical simulations of the experiment. [1]

BornAgain [2] is a multi–platform open–source project that aims at supporting scientists in the analysis and fitting of their GISAS data, both for synchrotron (GISAXS) and neutron (GISANS) facilities. The name of the software, BornAgain, indicates the central role of the distorted-wave Born approximation in the physical description of the scattering process. The software provides a generic framework for modelling 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 Rémi Lazzari [3], 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, Born-Again 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 (see figure 1 for an example of this last feature). Future extensions will include coverage of polarized GISANS for the investigation of magnetic domains.
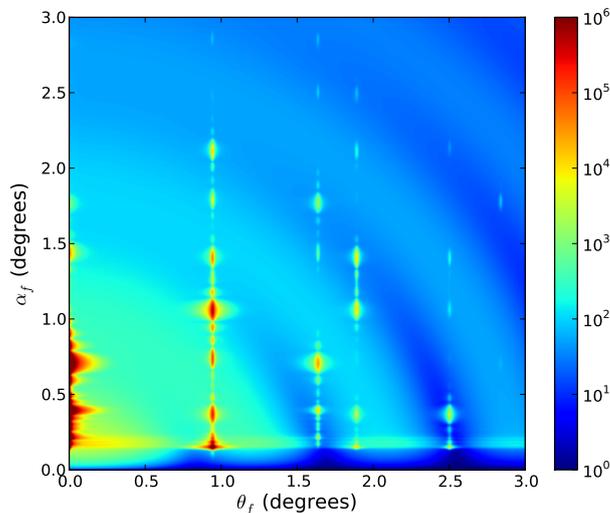


Figure 1: Simulation of grazing incidence scattering intensity for cylindrical mesocrystal islands on a substrate. The mesocrystals consist of an FCC structured self–assembly of spherical nanoparticles.

[1] G. Renaud, R. Lazzari, F. Leroy, *Probing surface and interface morphology with Grazing Incidence Small Angle X-Ray Scattering*, Surface Science Reports **64**, 255–380 (2009)

[2] BornAgain is available on http://apps.jcns.fz-juelich.de/bornagain

[3] R. Lazzari, *IsGISAXS: a program for Grazing–Incidence Small–Angle X–Ray Scattering analysis of supported islands*, J. Appl. Cryst. **35**, 406–421 (2002)

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