Grazing-incidence scattering is a powerful tool for the structural characterization of thin films, layered materials, nanoparticles depositions and many others [1]. However, a quantitative interpretation of the experimental results requires computational tools to perform numerical simulations and fitting algorithms. BornAgain is an open-source, multi-platform software that is more flexible and deals with more complex sample geometries than existing software.

Motivation

GISAS Experiments

Grazing-incidence small-angle scattering can deliver valuable information on the scattering density profile in both directions perpendicular and parallel to the sample surface. This same characteristic also makes the scattering data difficult to interpret and brings about the need for simulation and fitting tools.

Features of BornAgain

- Open-source, multi-platform software
- Inspired by established IsGisaxs program [2]: extended with support for multiple layers, interface roughness correlation, multiple types of nanoparticles in layers
- Physical model based on Distorted Wave Born Approximation
- Multiple fitting engines (from ROOT and GSL)
- Flexible, extendable framework in C++ (with python interface)
- Graphical User Interface for quick and easy sample manipulation and running of simulations (under development)
- Maintained by Scientific Computing Group of MLZ
- Professional approach to software development: short release cycles, issue- and bugtracking, version control, functional and unit tests, nightly builds, etc.

Scientific highlight

GISAXS experiment from a mesocrystalline system of self-assembled iron oxide spherical nanoparticles [3]:
- Mesocrystals have cylindrical shape and size about 1000 nm;
- Nanoparticles are spherical with mean radius 5 nm and assemble into an FCC lattice.

Comparison between experiment and simulation [4]:

Future Plans

BornAgain will be maintained by the Scientific Computing Group of MLZ. Its continued support will include providing bug fixes and new features at the user’s request. A Graphical User Interface and support for neutron polarization are already planned for implementation. Future users and interested people are all encouraged to stimulate further development by participating as beta users or co-developers of the project.

Info & Contact

Project website: http://apps.jcns.fz-juelich.de/bornagain

Workshop on Grazing Incidence Scattering Software on April 9-10, 2013:

registration ➔ http://apps.jcns.fz-juelich.de/doku/sc/giss_2013

References: