BornAgain: software for simulating and fitting small-angle scattering at grazing incidence

JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

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Grazing-incidence small-angle scattering
morphological characterization technique in reciprocal space

Suitable to probe
- both, hard and soft matter
- rough interfaces
- supported or buried nanostructures

Benefits
- surface-sensitive, non-destructive technique
- large area coverage
- tunable depth probe by changing incident angle
Grazing-incidence small-angle scattering
challenges of the data analysis

- Multiple reflections at interfaces due to small incident angle.
- Refraction shifts and distorts reciprocal space.
Grazing-incidence small-angle scattering

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\[ \tilde{q}_z = k \left( \sqrt{n^2 - \cos^2 \alpha_f} + \sqrt{n^2 - \cos^2 \alpha_i} \right) \]

Simulation required
Welcome to BornAgain

BornAgain is a software package to simulate and fit small-angle scattering at grazing incidence. It supports analysis of both X-ray (GISAXS) and neutron (GISANS) data. Its name, 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 modeling multilayer samples with smooth or rough interfaces and with various types of embedded nanoparticles.
BornAgain developers

Scientific Computing Group of MLZ. Group leader Dr. J. Wuttke.

Main developers

Gennady Pospelov
Walter Van Herck

Co-developers

Jan Burle
Jonathan Fisher
Marina Ganeva
Joachim Wuttke
Dmitry Yurov
Céline Durniak

Student interns

Rebecca Brydon
Sezer Karaca
Abhishek Khanna
Mohammad Mahadi Hasan
David Li
Ivonna Li

Anik Halder

Project was initiated by Prof. Th. Brückel
BornAgain project size: lines of code vs. time

Release 1.0
bornagainproject.org
Release 1.6
Fitting in GUI
Release 1.7
User meeting

PythonAPI
GUI
Unit Tests
Functional Tests
Core

Simulation of nanoparticles: shapes

- Anisotropic pyramid
- Box
- Cone
- Cone6
- Cuboctahedron
- Cylinder
- Ellipsoidal cylinder
- Full sphere
- Full spheroid
- Hemi-ellipsoid
- Prism3
- Prism6
- Pyramid
- Ripple1
- Ripple2
- Tetrahedron
- Truncated sphere
- Truncated spheroid
- Truncated cube
Simulation of nanoparticles: complex shapes

Core shell particles

Particles with size distribution
With possibility to link parameters

Particle compositions
collection of particles with fixed inter-particle distance
coherent interference

All can be rotated
Simulation of nanoparticles

Correlation between particles in different layers
Simulation of nanoparticles

Particles crossing layer interfaces
Simulation of nanoparticles

Dense particles: average material for Fresnel calculations
Simulation of nanoparticles

Graded layer approximation
Simulation of nanoparticles

Graded layer approximation
2D particle arrangement

Interference functions

- 1D lattice

- 2D lattice

- Radial paracrystal

- 2D paracrystal
Hexagonally ordered CoFeO$_4$ nanoparticles

Experiment: A. Qdemat, E. Kentzinger et. al., GALAXI

Model:

- nanoparticles in the hexagonal lattice
- local monodisperse approximation
Disordered Ag nanoparticles

Ag/PTFE/HMDSO nanocomposite, experiment at GALAXI

Model:
- nanoparticles with log-normal size distribution
- paracrystal interference, size-space correlation approximation
3D arrangements: mesocrystals

Model includes
- outer shape of the mesocrystal
- lattice vectors
- lattice basis (regular particles and their positions)
Nanostructure polymer films: mesocrystal


Real space

Lattice vectors

\[ \vec{a}_1 = \begin{pmatrix} L \\ 0 \\ 0 \end{pmatrix}, \quad \vec{a}_2 = \begin{pmatrix} 0 \\ d \\ 0 \end{pmatrix}, \quad \vec{a}_3 = \begin{pmatrix} 0 \\ \frac{1}{2} d \\ \frac{1}{2} d \tan \varphi \end{pmatrix} \]
Nanostructure polymer films: simulation


![Graph showing intensity as a function of qy and qz]
Iron oxide nanoparticles in FCC lattice

Elisabeth Josten, PhD thesis

Experiment (Soleil)

Simulation

Mesocrystal

M. Ganeva | BornAgain, ORNL, Oak Ridge, 2017
Large particles: aliasing problem

Rapidly oscillating signal at fixed points shows up as slow sinusoid

In GISAS simulation
Rapidly oscillating form factor of large particles leads to a significant variation of intensity over the detector bin.
Large particles: aliasing problem

Small cylinders
height = 10 nm
radius = 20 nm

Large cylinders
height = 1000 nm
radius = 2000 nm
**Interfaces with roughness**

Model from
Sinha et al 1988 (Phys.Rev.B 38, 2297) and

**Roughness is described by:**
RMS roughness $\sigma$
Hurst parameter $H$
Lateral correlation length $L_c$

For multilayer: cross-correlation length $L_h$
Specular and Off-specular geometry
Multilayer Ti/Pt resonator

H. Frielinghaus, et. al., NIM A 871 (2017) 72–76
Specular reflectivity (MARIA, MLZ)

H. Frielinghaus, et. al., NIM A 871 (2017) 72–76

![Graph showing specular reflectivity data](image)
Evanescent wave intensity

H. Frielinghaus, et. al., NIM A 871 (2017) 72–76

\[ I_e (z) = |\psi(z)|^2 = |R \cdot e^{ik_0 z} + T \cdot e^{-ik_0 z}|^2 \]
Off-specular scattering
H. Frielinghaus, et. al., NIM A 871 (2017) 72–76
Beam divergence and instrument resolution

Beam is defined via wavelength, incidence angles and intensity.

It is possible to define beam divergence and detector resolution function.
Magnetic nanoparticles + polarized neutrons

New in Release 1.9, July 2017

Model includes

- particle magnetization vector
- neutron beam polarization vector
- neutron analyzer direction, efficiency and transmission
Fitting in BornAgain: main features (1)

- Variety of minimization algorithms
  - **Library** | **Algorithm**
    - Minuit2 | Migrad, Simplex, Fumili, Scan
    - GSL | Fletcher-Reeves Conjugate Gradient Algorithm
    - | BFGS Conjugate Gradient Algorithm
    - | Levenberg-Marquardt Algorithm
    - TMVA | Genetic Algorithm

- Possibility to fit every sample parameter or their combination
  
  ```
  FitParameter("par1", 8.0*nm, limited(5.0, 15.0))
  radius = fun1(par1); lattice_length = fun2(par1)
  ```

- Various fit strategies (e.g. fix/release parameters)
Fitting in BornAgain: main features (2)

- Organizing different minimization algorithms into the chain
  ⇒ Genetic minimizer explores large parameter space, Levenberg-Marquardt finalizes location of minima

- Simultaneous fit of multiple datasets
  ⇒ Multiple experimental images can be fitted with one sample model

- Fitting along slices, masking certain areas of the detector image
Demo
Github workflow

github.com/scgmlz/BornAgain

GitHub cloud

BornAgain central repo

new in Release 1.7
Nov 2016

fork

Pull Request

Pull

Local computers

clone

Edits

M. Ganeva | BornAgain, ORNL, Oak Ridge, 2017
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Pull Request

Nightly builds
Functional tests
• 2 Mac OS
• 2 Win
• 6 Linux

fork

GitHub builds
• 1 Mac OS
• 1 Win
• 1 Linux

Pull

Local computers

clone

Edits

Code Review
BornAgain school and user meeting

- Tutorials at GISAXS2016 workshop, November 16–18, 2016, DESY, Hamburg
  4 groups x 12 students, 2 hours per group

- First BornAgain school and user meeting, November 21–22, 2016, Garching
  32 participants
BornAgain users

contributors

regularly making concrete suggestions
regularly finding bugs

writing us mails
regularly running BornAgain
generating user requests

appearing in download statistics
visiting web site
running BornAgain from time to time

1
Power users
3
Active users
> 50
Silent users
> 250
BornAgain citations

Data for 2017 were conservatively extrapolated to full year by multiplication with 12/5
Future plans

New 3D View in graphical user interface
Future plans

**Extend BornAgain for reflectometry (SINE2020)**

**Present**
- BornAgain allows to access full $R$, $T$ info
- Have simple specular peak depicted on top of 2D GISAS image
- Setup off-specular geometries
- Allows flexibly assemble models
- Infrastructure and user community

**Planned**
- Beam size effects
- Footprint correction
- Rocking curves, omega scans
- Material library, SLD profiles
- Roughness models
Future plans

Extend BornAgain for reflectometry (SINE2020)

ESS in-kind contribution
3 years FTE obtained

- Establish BornAgain as a standard software for ESS reflectomeres
- Provide fitting of GISAS, specular, off-specular data in a single framework
Thank you for your attention!

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