Transmission SAS options in BornAgain

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Overview

1. Overview of BornAgain

2. Self assembly of iron oxide nanoparticles

3. Python API example
History

- Project was initiated by Thomas Brückel and Sasha Ioffe
- Replacement of IsGISAXS (no longer supported)
- Support for polarized neutrons
- More flexible and extensible
- For both expert and novice users
- Scatter (Förster) and BornAgain
Physical model

- Based on Distorted Wave Born Approximation
- Unlimited number of layers
- Unlimited number of particles
- Interface roughness with optional cross-correlation

Coherent sum of four different scattering amplitudes. Only the first term is retained in the Born Approximation.
Sample modeling

- Tree of sample components
- Particle layouts:
  - Ensemble of particle shapes and their materials
  - Interference function: statistical information on the relative positions; for GISAS, the particles are ordered in the sample plane.

Polydisperse spheres on substrate
Instrument definition

- Beam: wavelength, intensity, incoming angles
- Detector: size, number of pixels, positions
- Polarization: beam polarization and analysis
- Distributions of wavelength and angles
Extensions for SAS (minimal)

- Instrument: 90° beam inclination
- 3d particle ordering:
  - Lattices: FCC, HCP, BCT, …
  - Peak shapes
  - Orientations: align specific q-axis with Miller indices of lattice
- Some adaptations in plotting \((Q_x - Q_y)\)
Self assembly of nanoparticles (WIP)


- Influence of magnetic field on self assembly
- From total disorder to crystalline structure

Disordered NPs form chains which assemble into supercrystal structures at high field strengths
Mixture of three models

The particles are core-shell spheres. The three ordering models are:

- Total disorder
- Partial order
  - Small finite paracrystal
  - Parameters: mean distance and peak width
- Body centered tetragonal order with two possible peak shapes
  - *3D Convolution*: convolution of an isotropic 3d Gaussian with a 2d von Mises-Fisher distribution
BCT peak shape models

- 3d von Mises-Fisher
- Convolution 2d and 3d von Mises-Fisher
- Convolution 3d Gauss with 2d von Mises-Fisher
Unordered nanoparticles at 0 T

Total disorder
Partially ordered nanoparticles at 0.1 T

80% disorder, 20% partial order
Partially ordered nanoparticles at 0.5 T

10% disorder, 55% partial order, 35% BCT (factorized)
Partially ordered nanoparticles at 1 T

20% partial order, 80% BCT (factorized)
Fully ordered nanoparticles at 3 T

Mostly BCT (3d convolution); 4m sample detector distance
Rotating FCC lattice of spherical nanoparticles.
Fitting spherical core-shell particles.
Overview of BornAgain
Self assembly of iron oxide nanoparticles
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More information on the BornAgain website

http://www.bornagainproject.org/