

BornAgain: A software to simulate and fit GISAS

Jan Burle, Céline Durniak, Jonathan M. Fisher, Marina Ganeva, Gennady Pospelov,
Walter Van Herck, Joachim Wuttke

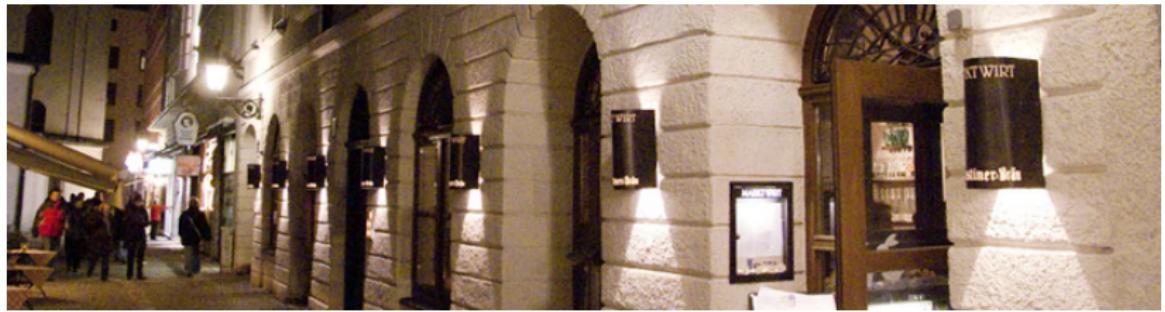
Garching, 21 nov 2016

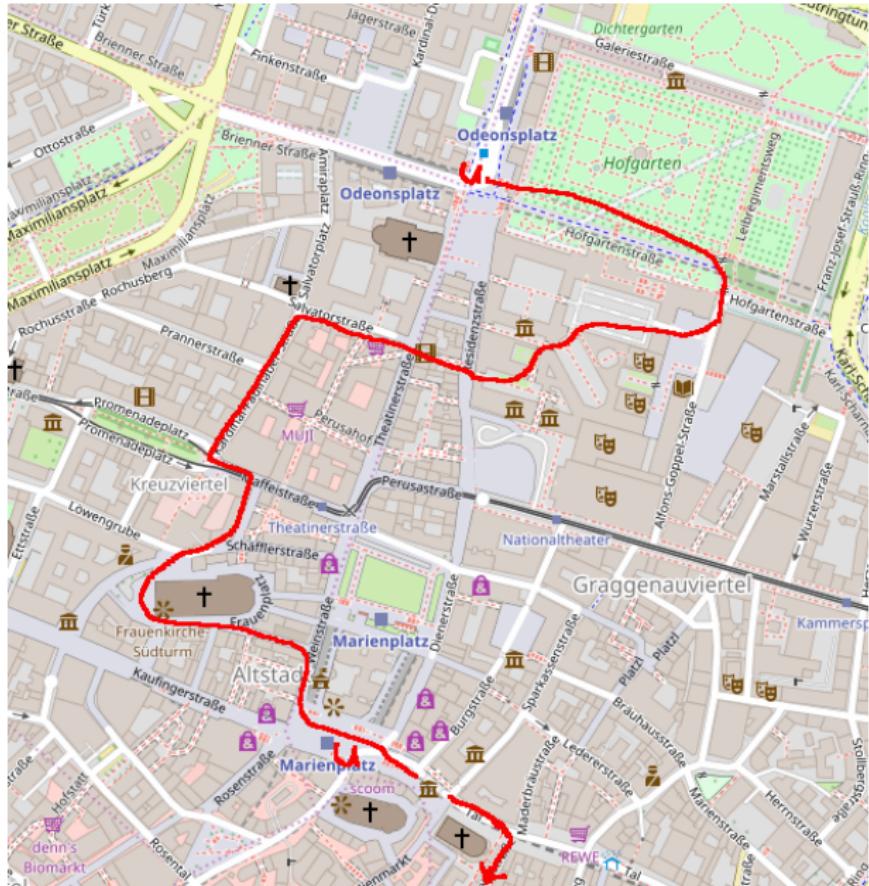
MLZ is a cooperation between



Technische Universität München







Conference Dinner

Today 19h45, Marktwirt, Heiliggeiststraße 2

leave GATE	18h10	18h50
U6 Garching-Forschungszentrum	18h26	19h06
U6 Garching	18h29	19h09
U6 Garching-Hochbrück	18h31	19h11
U6 München-Odeonsplatz	18h50	
U6 München-Marienplatz		19h32
meet at Marktwirt	19h45	19h45

Conference Program

Mon 14-17 BornAgain introduction and tutorial

17-18 Poster session

Tue 9-13 BornAgain tutorial ctd

13-14 Lunch offered

14-17 User talks, discussion

User Talks

Tuesday 14h

Hard matter

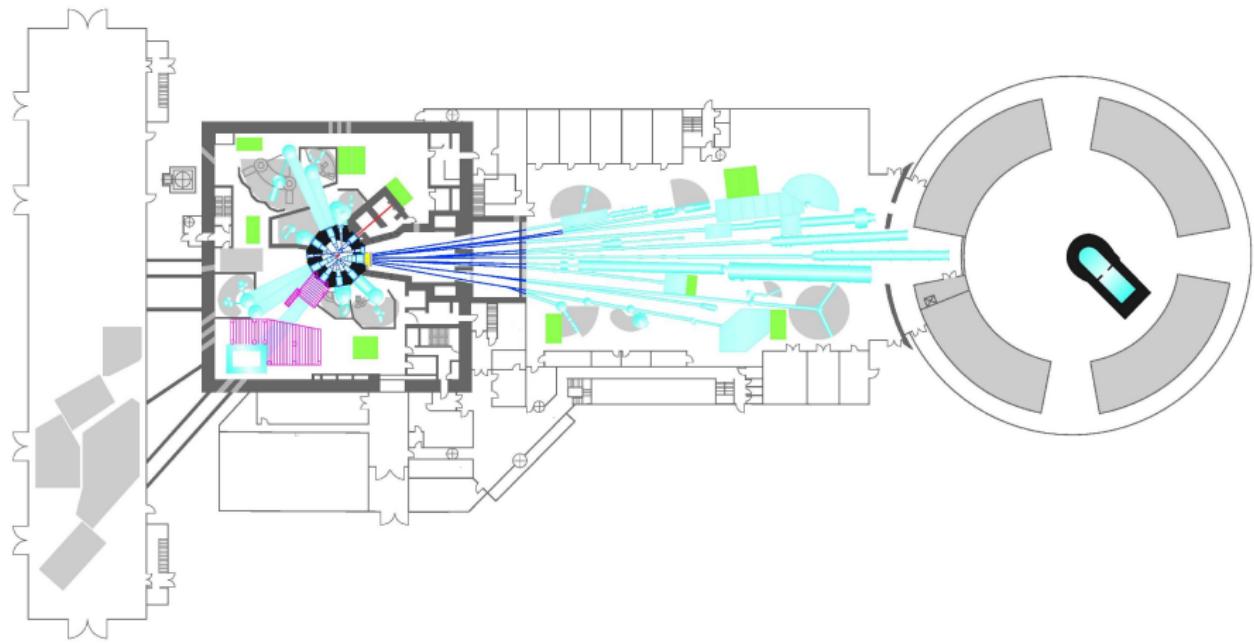
- | | |
|----------|---|
| Emmanuel | Polarized GISANS from lateral spin correlations |
| Dieter | Dy/Y multilayers and off-specular magnetic scattering |
| Henrich | Resonator |
| Mika | Reconstruction of Structure Parameters |

Soft matter

- | | |
|--------|--|
| Deniza | Geometrical structure of ultrasmall Au9 nanoclusters |
| Jacqui | Dye aggregation in dye-sensitized solar cells |
| Olaf | Reverse hexagonal phase of self-assembled lipids |

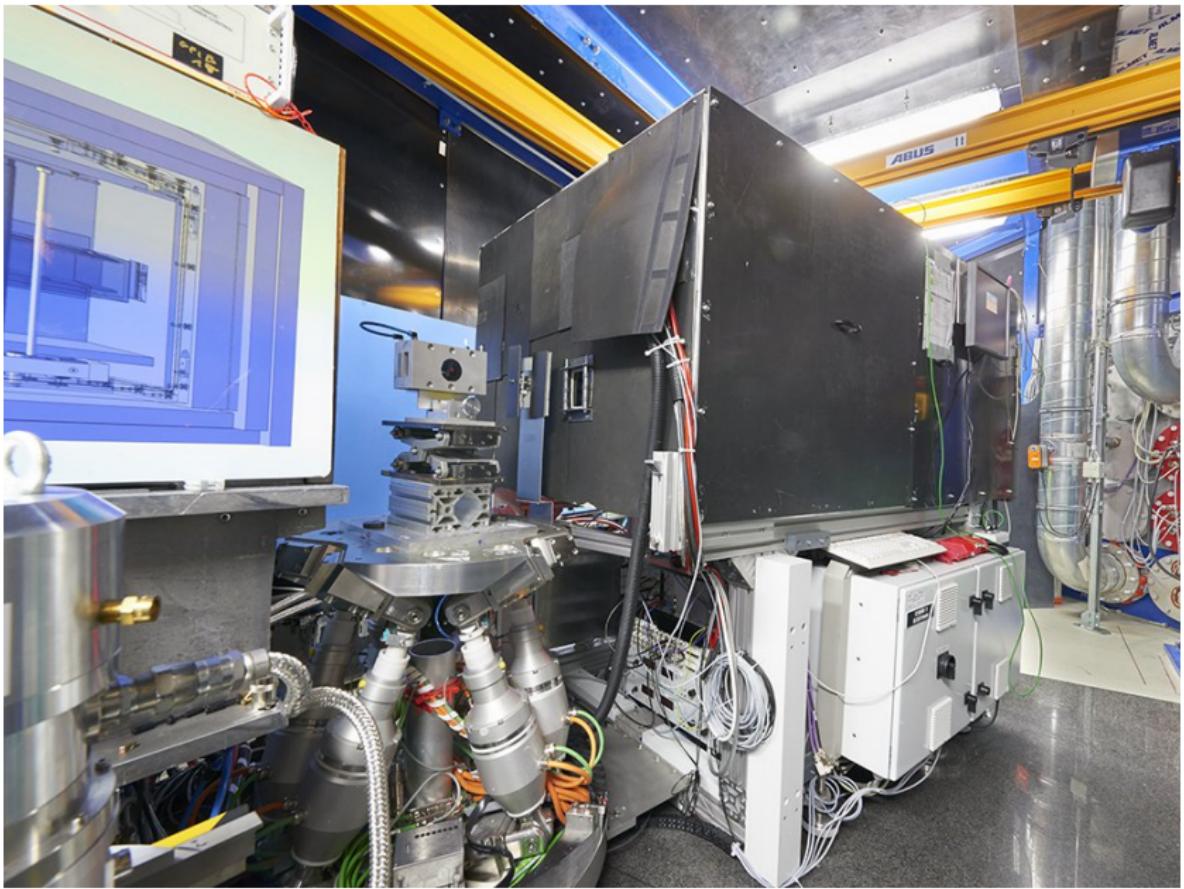
Final discussion

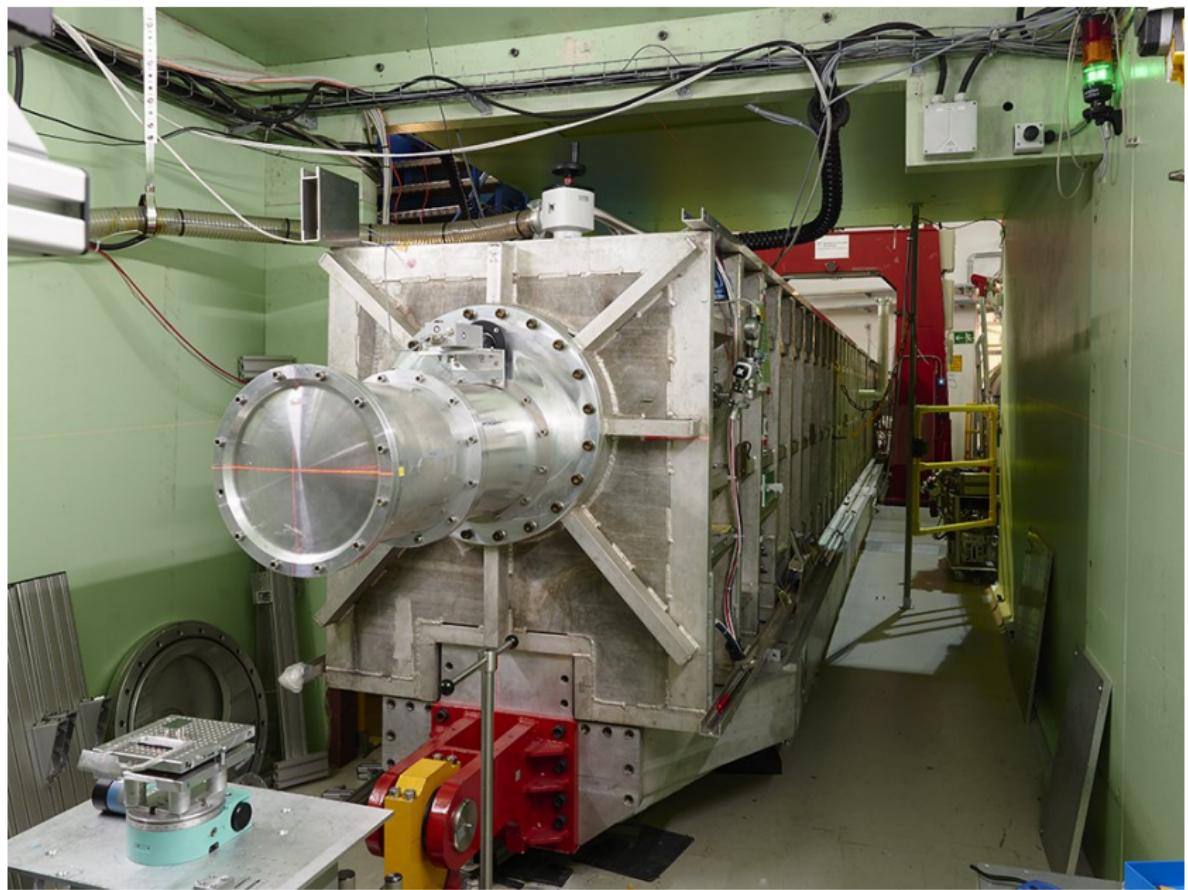
- | | |
|---------|--------------------------------|
| Artur | Real-world challenges in GISAS |
| Joachim | Outlook |











research reactor FRM II at Garching near Munich

scientific use through Heinz Maier-Leibnitz Zentrum (MLZ)



Scientific Computing Group at MLZ Garching

Mission:

- develop/adapt/maintain software
for data reduction and analysis
at neutron scattering instruments of MLZ

Staff:

- five scientist-developers on core budget
- one position from EU SINE2020
- future collaborations with Univ Erlangen, ESS Lund

Initial projects:

- Data reduction for time-of-flight spectrometers
- Data reduction for materials diffractometer
- Simulation and fitting of GISAS

SINE2020

Science & Innovation with Neutrons in Europe in 2020



User Name Password
[Login](#) | [Lost Password](#) | [Register](#)

ABOUT R&D ACTIVITIES INDUSTRY TRAINING NEWS AND MEDIA

Search

Data Treatment Software

Coordinator: [✉ Thomas Holm Rod \(ESS\)](#)

Partners: ESS, ILL, STFC, PSI, Juelich, CEA, Universita' degli studi di Parma

Overview

This WP has two main objectives with respect to users:

- Straightforward generation of scientific results for non-expert and industry users that are either directly publishable or can be used for creating new innovative products.
- Data treatment software ready for users at ESS in 2020 – users will be familiar with the software and able to produce high-impact results from day one.

► CHEMICAL DEUTERATION

► CRYSTAL GROWTH

► SAMPLE ENVIRONMENT

► E-TOOLS

► DETECTORS

► DATA TREATMENT

 ▶ News

 ▶ Meetings

International division of tasks

SINE2020 workpackage 10: data treatment software

Technique	Facility	Software
Reflectometry	MLZ	BornAgain
QENS	ISIS	Mantid/Vates
Atomistic modelling	ILL	nMoldyn, DFT
SANS	ESS	SASView
Imaging	PSI	MuhRec/KipTool

Wishlist

Scientific software should be

- correct
- efficient
- easy to use
- documented (*and have open code*)
- adaptable, extensible (*also by users*)
- long-term available (*in extremis* by forking)

Scientific software development standards

Each software project should have

- clear licence status
- institutional support commitment
- no personal ownership, no dependence on single person
- well-chosen dependence on standard libraries and tools
- version control
- unit and functional test coverage
- automated builds and tests for all supported platforms
- web home page, mailing list, issue tracker
- short release cycles
- channels for user feedback

why GISAS simulation software?

- fit data
- support semi-quantitative or qualitative data analysis
- train experimentalists' intuition

why new GISAS simulation software?

to simulate

- multilayers
- polarized scattering
- magnetic domains

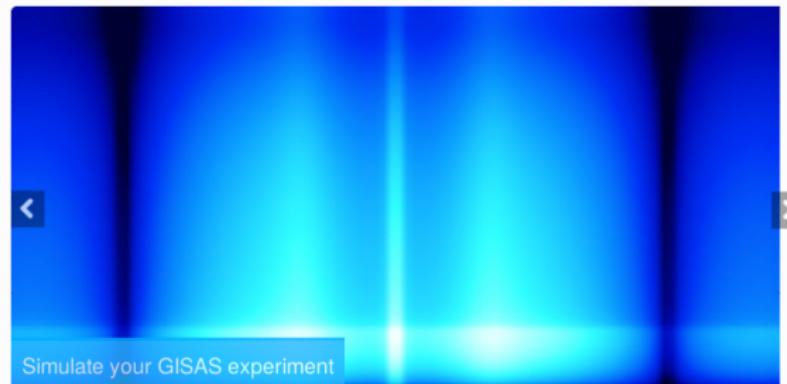
to support

- polarized neutron reflectometer MARIA
- X-ray reflectometer GALAXI
- in-house research
- user community at large



BornAgain

Simulate and fit grazing incidence small angle scattering

[Home](#)[Screenshots](#)[Download](#)[Documentation](#)[Contact](#)[Forums](#)[About](#)

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.

Support

register to receive announcements or post to the forum

USER LOGIN

Username *

Password *

- [Create new account](#)
- [Request new password](#)

Download server

Wiki Tickets Downloads

MLZ
Heinz Maier-Leibnitz Zentrum

Scientific Computing

data analysis software for neutron scattering

Download directory /src/BornAgain

Name	Last modified	Size
◀ Parent Directory		-
experimental	15-Nov-2016 12:43	-
old	15-Nov-2016 12:42	-
BornAgain-1.7.0-macosx64-10.9+.dmg	14-Nov-2016 17:04	21M
BornAgain-1.7.0-win64.exe	14-Nov-2016 14:41	18M
BornAgain-1.7.0.tar.gz	14-Nov-2016 16:49	78M
BornAgainManual-1.7.0.html	15-Nov-2016 12:47	8.7M
BornAgainManual-1.7.0.pdf	15-Nov-2016 12:47	12M
CHANGELOG	15-Nov-2016 12:46	52K

Source repository

Get involved: report issues, propose patches

The screenshot shows a GitHub repository page for `scgmlz / BornAgain`. At the top, there are tabs for `This repository`, `Search`, `Pull requests`, `Issues`, and `Gist`. On the right, there are icons for notifications, adding a star, and forking the repository.

The repository name `scgmlz / BornAgain` is displayed, along with statistics: `7,955 commits`, `2 branches`, `34 releases`, `8 contributors`, and a license bar for `GPL-3.0`.

A brief description states: "A software to simulate and fit neutron and x-ray scattering at grazing incidence. <http://www.bornagainproject.org> — Edit".

Your recently pushed branches section shows a branch `jwuttke:src_j3` (about 1 hour ago). There is a green button to `Compare & pull request`.

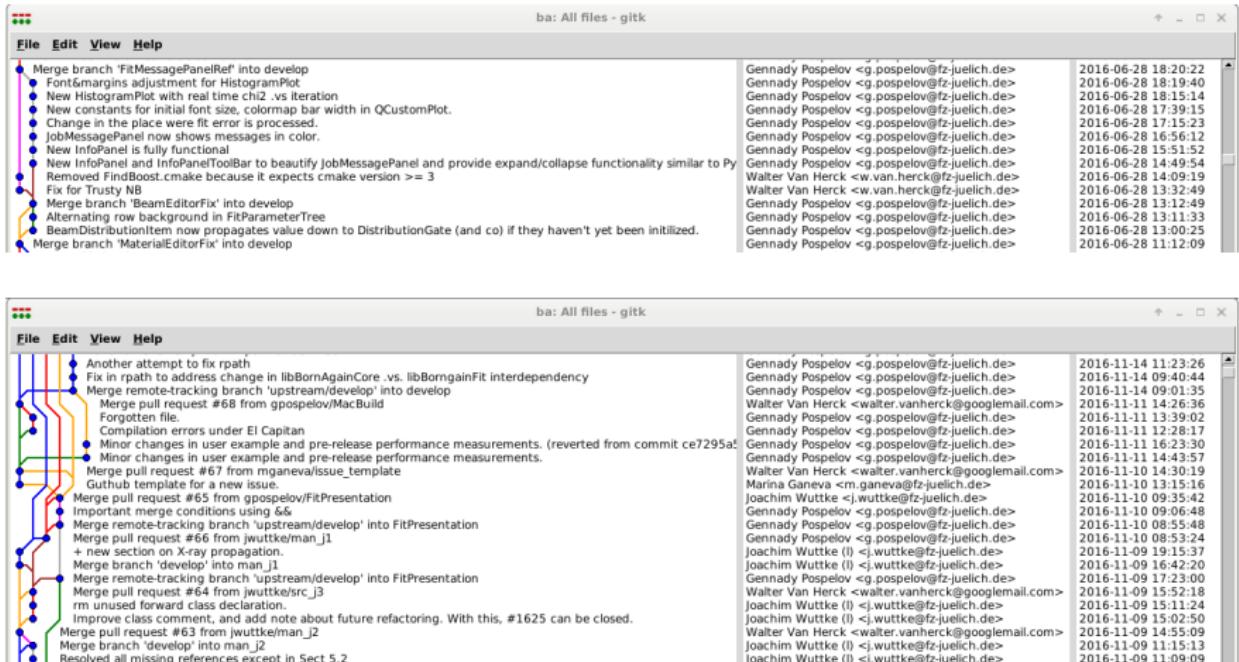
The main commit list shows the following recent commits:

- gpospelov** committed on GitHub Merge pull request #74 from waltervh/release-1.7.0 ...
- .github** Github template for a new issue.
- .travis** Travis testing disabled for MacOS builds
- Core** Remove default parameter value for total transmission of analyzers
- Doc** Remove obsolete generation of `findBornAgain.cmake` and `BAVersion.h` in ...
- Examples** Minor fix to Python fitting example and added performance measurement
- El Capitan** Compilation errors under El Capitan

On the right side, there is a `Clone with HTTPS` section with the URL `https://github.com/scgmlz/BornAgain.git` and a `Download ZIP` link.

Source repository

viewed with gitk



Internal issue tracker

public read access

Home Projects Help Sign in Register

BornAgain

Search:

Overview Activity Roadmap Issues Calendar Wiki Repository

Issues

Filters Status open Add filter ▾

Options Apply Clear

#	Tracker	Status	Priority	Subject	Assignee	Target version	% Done
1650	Refactoring	Rfc	Normal	Designation "ROOT" (or "Root" or "BA_ROOT") should not be used for code other than CERN ROOT			
1649	Refactoring	New	Normal	Ensure consistent use of ambientMaterial			
1646	Bug	New	Normal	Reversed order numpy array			
1645	Envelope task	In Progress	High	== Graded layer and cross-layer particles ==	Sprint 33		
1644	Documentation	New	Normal	"User Login" block on homepage should explain _why_ to create account			
1641	Bug	New	Normal	histogram2d test fails under certain configurations			
1640	Configuration	Backlog	Normal	Doxygen generation on apps server not compatible anymore with links to API			
1639	Bug	Sprint	Normal	GUI: crash if fitting parameter removed	Sprint 33		
1638	Documentation	Backlog	Low	Manual: Improve / restore side bar navigation			
1637	Bug	Backlog	Normal	GUI: just loaded fitting project appears as already changed			
1636	Bug	New	High	Unexpected wavelength depent intensity Roughness ue. Darstellung			

Issues

View all issues
Summary
Calendar

Custom queries

assigned to me
authorized by me
by priority
by status
by tracker
by tracker, current sprint
treeview

The reference

IsGISAXS by Rémi Lazzari



IsGISAXS: a program for grazing-incidence small-angle X-ray scattering from supported islands

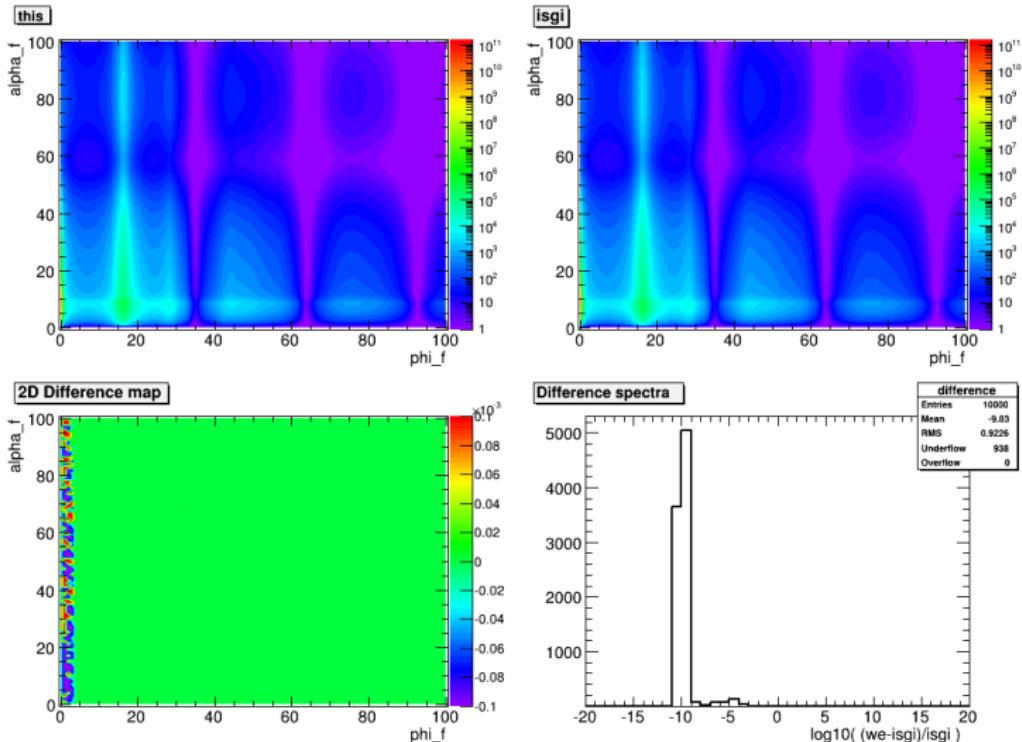
R Lazzari - Journal of Applied Crystallography, 2002 - scripts.iucr.org

This paper describes a Fortran program, IsGISAXS, for the simulation and analysis of grazing-incidence small-angle X-ray scattering (GISAXS) of islands supported on a substrate. As is usual in small-angle scattering of particles, the scattering

Cited by 378 Related articles All 5 versions Import into BibTeX Save

Validation

BornAgain vs IsGISAXS



BornAgain functionality

Release 1.7 of Nov 15

Sample modelling:

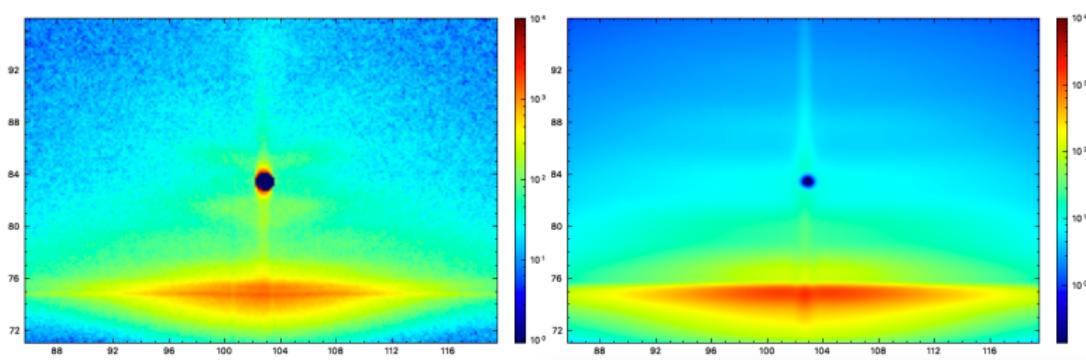
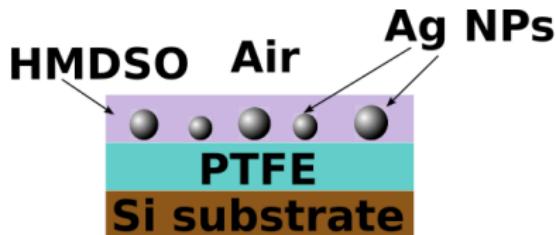
- IsGISAXS almost fully replicated
- arbitrary number of layers
- arbitrary particle layouts (shape \otimes interference fct)
- compound particles
- mesocrystals
- polarized neutron propagation
- scattering by magnetic nanoparticles
- 2d fitting, masking
- off-specular scans

Usability:

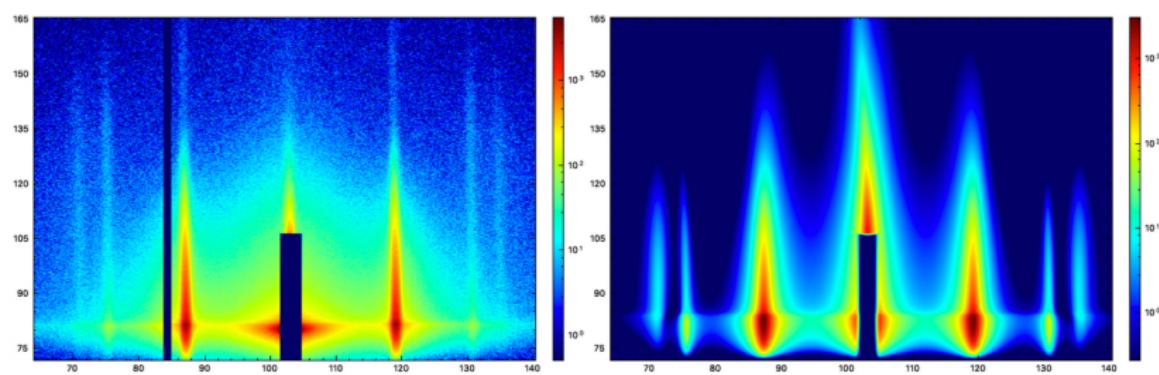
- can be run from C++, Python, or GUI
- construct model in GUI, export to Python
- many examples, growing manual

HMDSO/Ag/PTFE nanocomposites

Layers have roughness. Nanoparticles have lognormal size distribution.

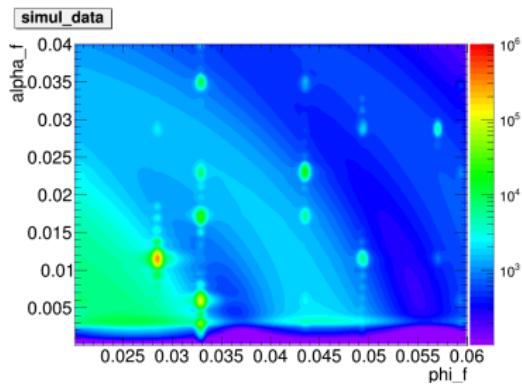
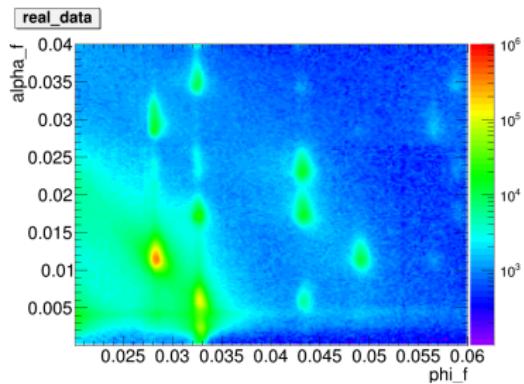
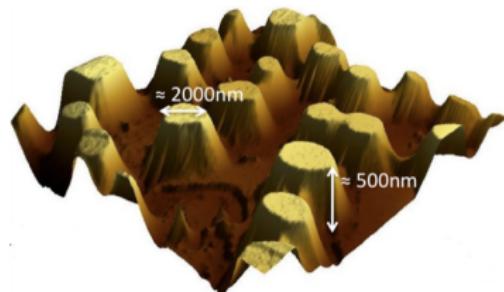


Co nanodots

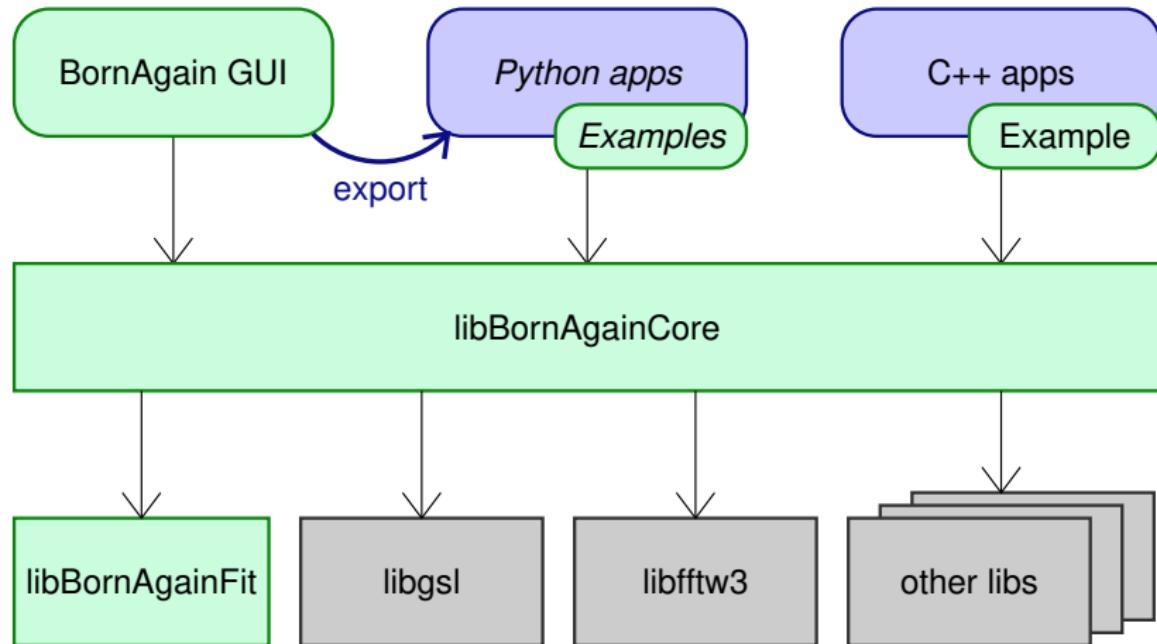


Mesocrystal assembly

2D random assembly
of fcc mesocrystals of size $\sim 1 \mu\text{m}$
of spherical particles of size 5 nm

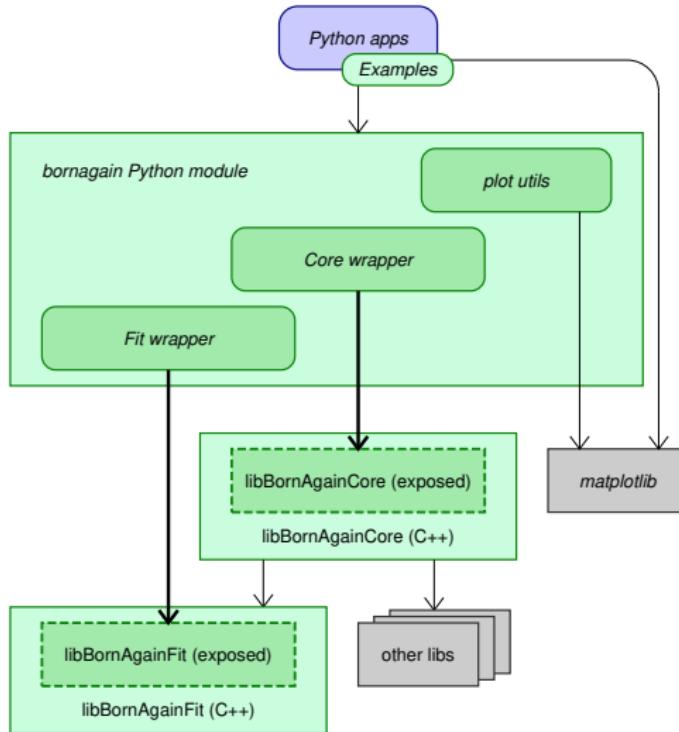


Architecture



Python module BornAgain

import bornagain as ba



Basic simulation under Python

```
import bornagain as ba

sample = ba.MultiLayer()
...

simulation = ba.GISASSimulation()
simulation.setBeamParameters(
    1.0*angstrom, 0.2*deg, 0.0*deg)
simulation.setDetectorParameters(
    100, -1*deg, 1*deg, 100, -1*deg, 1*deg)
simulation.setSample(sample)

result = simulation.runSimulation()

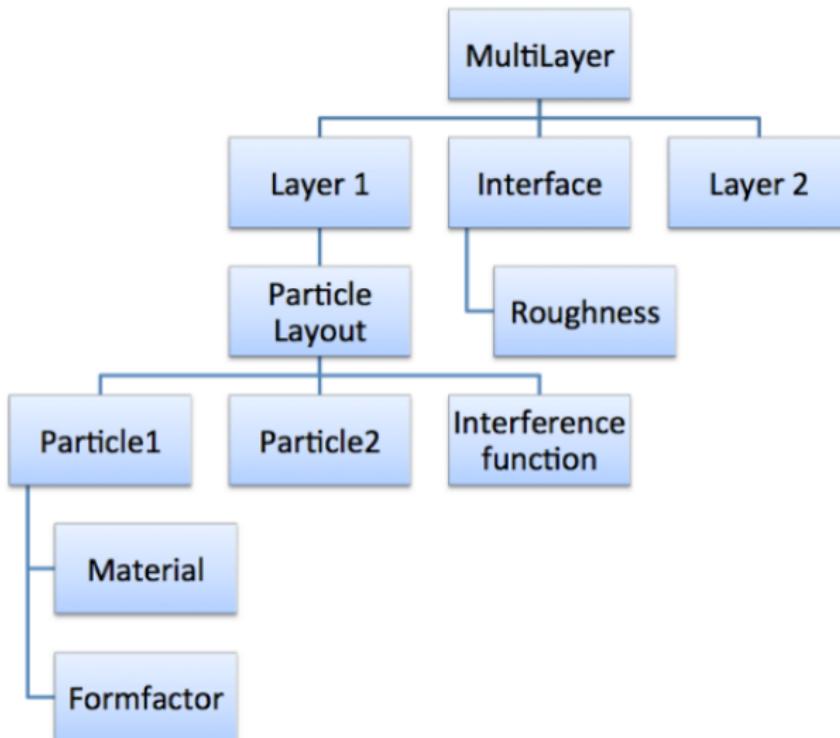
ba.plot_intensity_data(result)
```

Hierarchical data structure

GISASSimulation

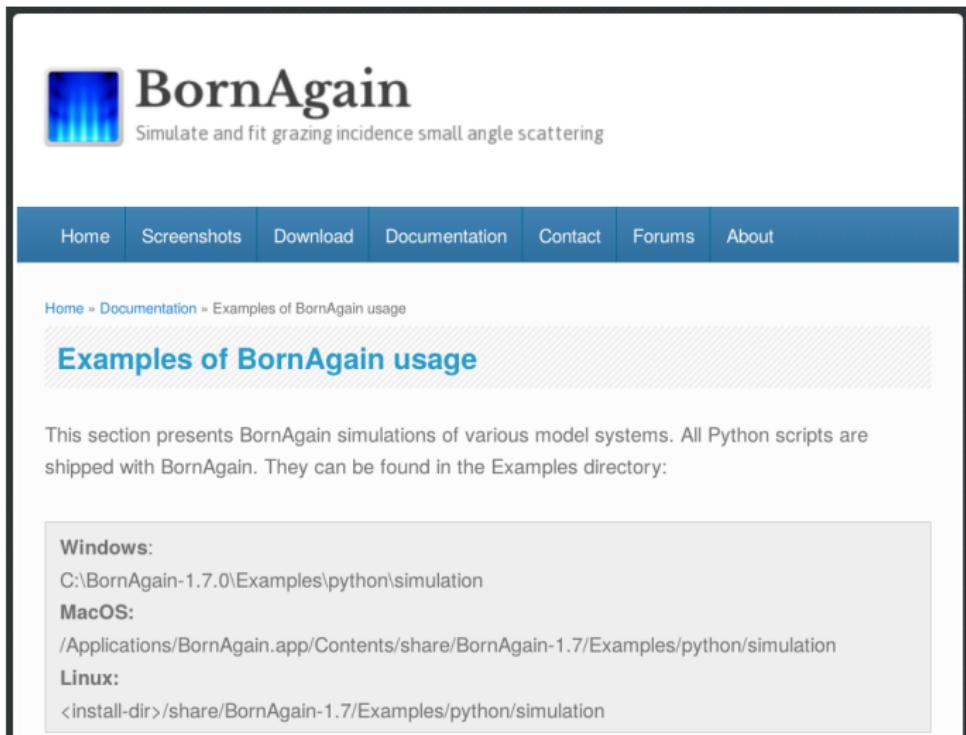
- Beam
- Detector
- Sample
 - Interface(s)
 - Roughness
 - Layer(s)
 - ParticleLayout
 - Particle(s)
 - Material
 - FormFactor

Hierarchical sample model



Application programming interface (API)

documented through usage examples



The screenshot shows a web page for 'BornAgain'. At the top left is a blue square icon with vertical white bars of varying lengths. To its right is the word 'BornAgain' in a large, bold, black sans-serif font. Below this, in a smaller, gray font, is the text 'Simulate and fit grazing incidence small angle scattering'. A horizontal navigation bar below the title contains links for Home, Screenshots, Download, Documentation, Contact, Forums, and About. The main content area has a light gray background. At the top of this area, there is a breadcrumb navigation: 'Home » Documentation » Examples of BornAgain usage'. Below this is a section header 'Examples of BornAgain usage' in a large, bold, blue font. The text within this section reads: 'This section presents BornAgain simulations of various model systems. All Python scripts are shipped with BornAgain. They can be found in the Examples directory:'. Inside a light gray box, there are four entries: 'Windows:', 'MacOS:', 'Linux:', and their corresponding file paths. The Windows path is 'C:\BornAgain-1.7.0\Examples\python\simulation'. The MacOS path is '/Applications/BornAgain.app/Contents/share/BornAgain-1.7/Examples/python/simulation'. The Linux path is '<install-dir>/share/BornAgain-1.7/Examples/python/simulation'.

Home » Documentation » Examples of BornAgain usage

Examples of BornAgain usage

This section presents BornAgain simulations of various model systems. All Python scripts are shipped with BornAgain. They can be found in the Examples directory:

Windows:
C:\BornAgain-1.7.0\Examples\python\simulation

MacOS:
/Applications/BornAgain.app/Contents/share/BornAgain-1.7/Examples/python/simulation

Linux:
<install-dir>/share/BornAgain-1.7/Examples/python/simulation

Application programming interface (API)

selective reference in User Manual, Part II

```
class Layer {
    Layer();
    Layer(const IMaterial& material, double
          thickness=0);
    void setThickness(double thickness);
    void setMaterial(const IMaterial& material);
    void addLayout(const ParticleLayout&
                   decoration);
};
```

Application programming interface (API)

full reference automatically generated by Doxygen

BornAgain 1.7.0

Main Page User API Full C++ API File List Search

Class List Class Index Class Hierarchy

BornAgain

User API

Full C++ API

Class List

Class Index

Class Hierarchy

File List

Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

[detail level 1 2]

DetectorFunctions	Contains set of detector-related convenience functions
Exceptions	
FileSystem	Utilities to deal with file system
Geometry	
MathFunctions	Various mathematical functions
MSG	Sets of logging utilities
Numeric	Floating-point epsilon, tolerances, almost-equal
StandardSimulations	Standard pre-defined simulations
Utils	
AdjustMinimizerStrategy	Strategy modifies minimizer settings before running minimization round
AngularPixelMap	
AttLimits	Defines limited/free attribute of fit parameter and provides coupling between them
Attributes	Attributes for a fit parameter
Basic2DLatticeBuilder	Builds sample: 2D lattice with arbitrary angle and different lattice length_1 and length_2
Basic2DParaCrystalBuilder	Builds sample: basic two dimensional paracrystal with various probability distribution functions (PDFs)
BasicVector3D	Three-dimensional vector template, for use with integer, double, or complex components
Beam	Ideal collimated beam defined by wavelength, direction and intensity

Three parts of any simulation

```
# construct the model
simulation = ba.GISASSimulation()
simulation.setBeamParameters(
    1.0*angstrom, 0.2*deg, 0.0*deg)
simulation.setDetectorParameters(
    100, -1*deg, 1*deg, 100, -1*deg, 1*deg)
simulation.setSample(...)

# run the simulation
result = simulation.runSimulation()

# analyse the outcome
ba.plot_intensity_data(result)
```

Distorted-Wave Born Approximation

leaves freedom in choice of distorted wave

Schrödinger equation, splitted for perturbation expansion:

$$\left\{ \nabla^2 + \frac{2m\omega}{\hbar} - 4\pi \bar{V}(\mathbf{r}) \right\} \psi(\mathbf{r}) = 4\pi \delta V(\mathbf{r}) \psi(\mathbf{r})$$

\bar{V} = const: plane-wave Born expansion

$\bar{V}(\mathbf{r})$ slowly varying: distorted-wave Born expansion

$\bar{V}(z)$ slowly varying: GISAS-DWBA

$\bar{V}(z)$ step function: standard model in IsGISAXS, FitGISAXS, ...

Computing scattering intensities in DWBA

Precompute R & T coefficients

Loop over detector bins:

- Compute transmission to detector

- Compute scattering from rough interfaces

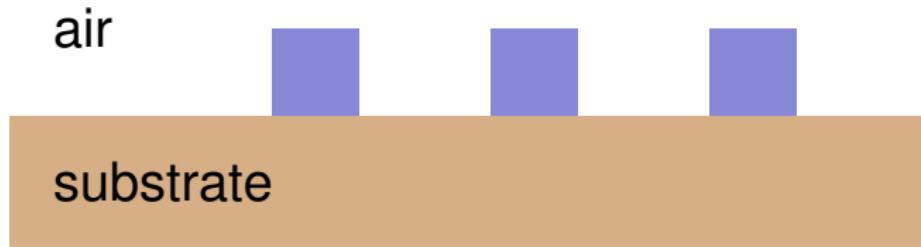
- Compute scattering from particle layout

Getting the hierarchical data to work

just a few out of many function calls

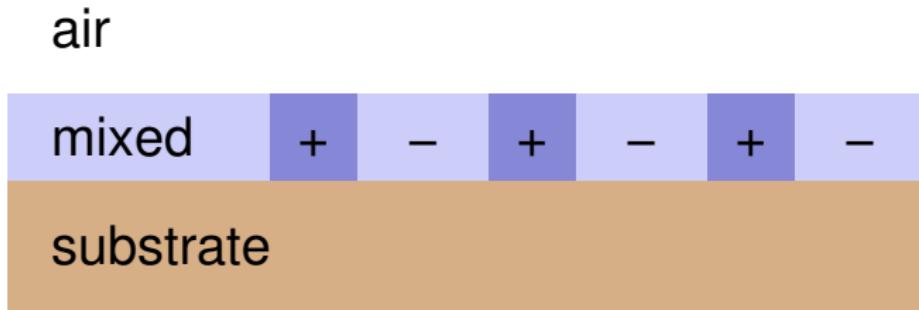
```
GISASSimulation.runSimulation()
- MainComputation.run()
- MainComputation.collectRTCoefficientsScalar()
  ... - SpecularMatrix.execute(sample, k, coeffs)
- Multilayer.getLayer(i)
  - Layer.getThickness()
  - Layer.getRefractiveIndex()
  - Layer.getLayout(j)
    - ParticleLayout.getParticle(k)
    - ParticleLayout.getAbundanceOfParticle(k)
      - Particle(s).getFormFactor()
        - Material.getRefractiveIndex()
        - FormFactor.evaluate_for_q(q)
```

Decorated air layer



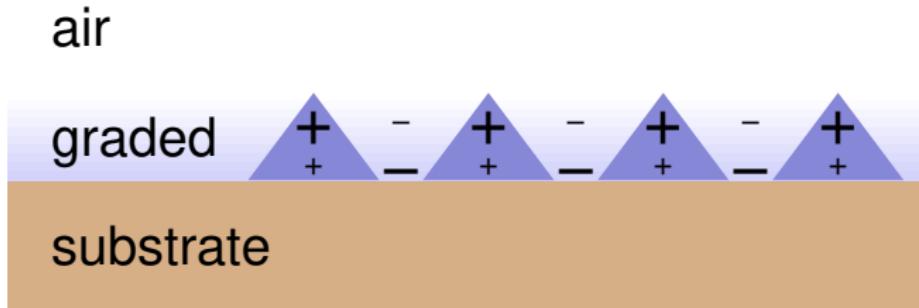
Decorated air layer

improve choice of \bar{V}



Decorated air layer

further improvement: graded $\bar{V}(z)$



Possible approaches:

- 5–20 homogeneous slices
- Airy function for $n^2 \sim a + bz$
- Numeric integration for any $n(z)$

Requires major refactoring

move ParticleLayout from Layer to MultiLayer level

