# STRUCTURAL CHARACTERIZATION OF QUANTUM DOT LATTICES BY GISAXS: MODELS AND SOFTWARE PACKAGE GisaxStudio

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## INTRODUCTION

**GISAXS (grazing incidence small angle x-ray scattering) is a powerful method for structural characterization of materials. Although GISAXS measurements are very simple, the models describing the scattered intensity are often missing as the intensity strongly depend on the specific structure of the material. Here we present models [1,2] and computer program *GisaxStudio* for the structural characterization of nanostructured materials consisting of different quantum dot lattices by GISAXS. They enable the determination of the shape and arrangement properties of different nano-objects embedded in a matrix as well as their statistical distributions. *GisaxStudio* is a modular, multi-platform program written in Java programming language, featuring a graphical user interface, built-in optimization algorithms and visualization. The package contains two classes of models. The first one: *GisaxStudio-3dLattice* is aimed for the analysis of the materials consisting of 3D lattices of quantum dots or nanoparticles. The models included there are suitable for the materials produced by some of self-assembly processes. The second one: *GisaxStudio-iBeaM*, is suitable for the analysis of the materials modified by ion beams and all similar ones.**

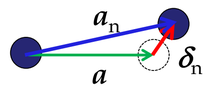
## MODELING OF GISAXS INTENSITY DISTRIBUTIONS

$$I(Q) = A|\delta\varrho|^2|t_i t_f|^2 \left\langle \sum_{R,R'} \Omega_R(\boldsymbol{q})\Omega^*_{R'}(\boldsymbol{q}) \mathrm{e}^{-\mathrm{i}(\boldsymbol{q}.\boldsymbol{R}-\boldsymbol{q}^*.\boldsymbol{R}')} \right\rangle .$$

**For 1D case we assume three possible ordering types:**

1. SHORT RANGE ORDERING (**SRO**):

$$\boldsymbol{R}_n = n\boldsymbol{a} + \sum_{j=1}^{n} \boldsymbol{\delta}_j = n\boldsymbol{a} + \boldsymbol{D}_n,$$

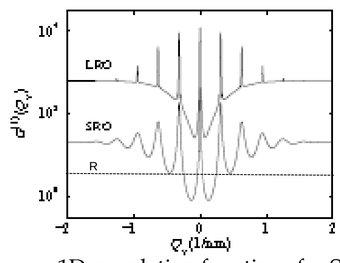



2. LONG RANGE ORDERING (**LRO**):

$$\boldsymbol{R}_n = n\boldsymbol{a} + \boldsymbol{D}_n = n\boldsymbol{a} + \boldsymbol{\delta}_n,$$

3. RANDOM POSITIONS (**R**):

$$\boldsymbol{R}_n = \boldsymbol{\rho}_n,$$




1D correlation functions for SRO and LRO models.

**For n-dimensional QD lattice different combinations of LRO, SRO and R may occur:**

**3D example:** $R_{n_1,n_2,n_3} = n_1\boldsymbol{a}^{(1)} + n_2\boldsymbol{a}^{(2)} + n_3\boldsymbol{a}^{(3)} + \boldsymbol{D}^{(1)}_{n_1} + \boldsymbol{D}^{(2)}_{n_2} + \boldsymbol{D}^{(3)}_{n_3},$

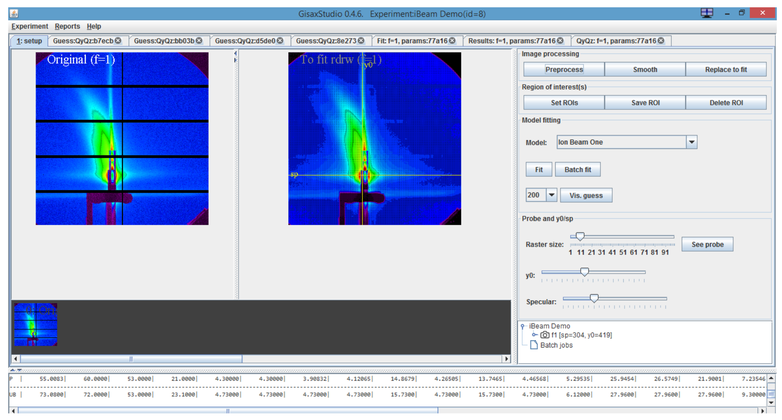
**Disorder parameters: $\sigma^{(1)}_{x,y,z}$, $\sigma^{(2)}_{x,y,z}$, $\sigma^{(3)}_{x,y,z}$**

**Details given in Refs. [1,2]**

## SOFTWARE PACKAGE *GisaxStudio*:

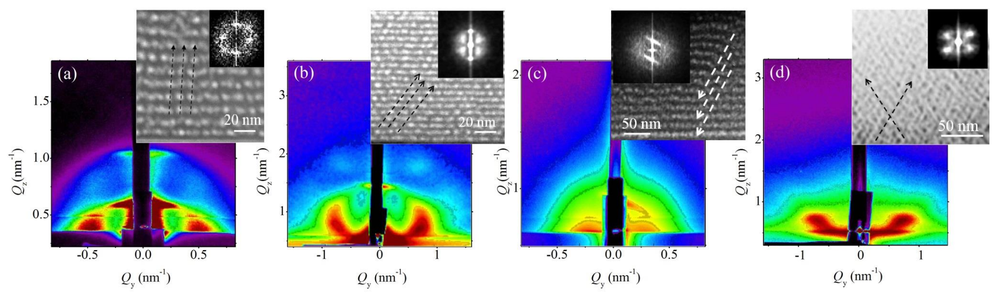

**Software package *GisaxStudio* contains two families of models**: -*3dLattice* for the analysis of three-dimensional quantum dot lattices formed by different self-assembly processes and ***-iBeaM*** which is suitable for the analysis of GISAXS intensity distributions measured on ion-beam modified materials. The program is freely available at the site: http://homer.zpr.fer.hr/gisaxstudio.

- ✓ IMAGE PROCESSING
- ✓ DIFFERENT MODELS
- ✓ SIMULATION
- ✓ FITTING
- ✓ BATCH FIT
- ✓ SAVING TO DATABASE



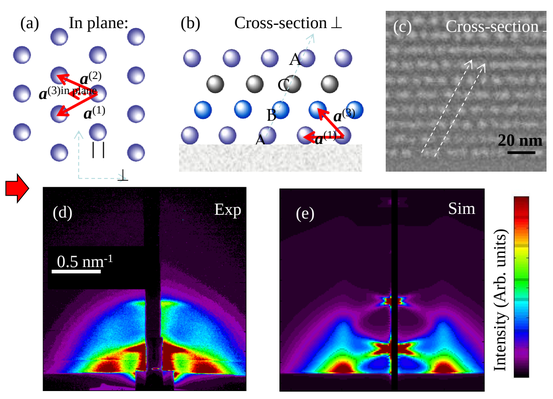

**Main window of *GisaxStudio-iBeaM***

## *GisaxStudio-3dLattice:* 3D QUANTUM DOT LATTICES



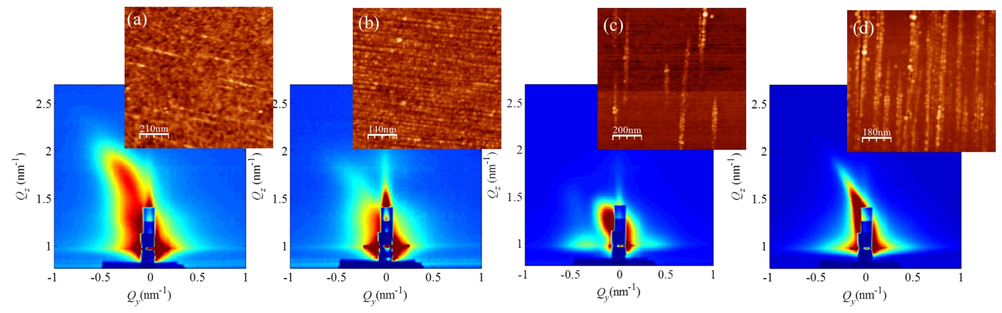

**Surface tracks: examples showing different structural properties.** GISAXS intensity distributions and corresponding TEM images (insets) measured on Ge quantum dots obtained by different self-assembly processes . **A theory is developed in Ref. [1], models 1-3.**

MODEL 1: SELF-ASSEMBLY IN ALL DIRECTIONS
MODEL 2: TEMPLATED SELF-ASSEMBLY
MODEL 3: SELF-ASSEMBLY IN MULTILAYERS



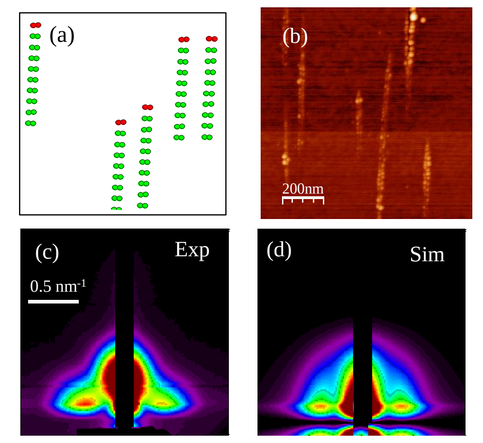

**Example of GISAXS data analysis using the MODEL SELF-ASSEMBLY IN MULTILAYERS.** (a),(b) the assumed ordering of quantum dots, (c) TEM cross-section of the sample, (d) experimentally measured GISAXS map and (e) simulatied map used the parameters obtained by fit.

## *GisaxStudio-iBeaM:* SURFACE TRACKS (ion beam irradiation)




**Surface tracks: examples showing different structural properties.** GISAXS intensity distributions and corresponding AFM images (insets) measured on Ge+ITO films irradiated with different ion types and doses under angle of 1 deg. **A suitable theory for the description of the GISAXS data is given in Ref. [2].**

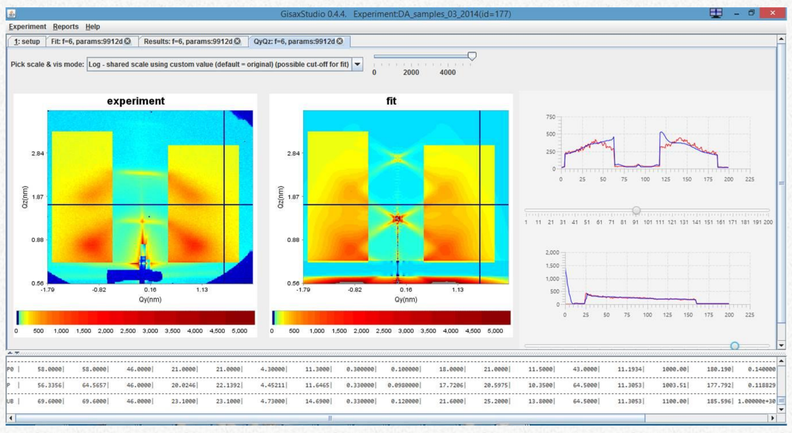
MODEL 1: UNCORRELATED SINGLE TRACKS
MODEL 2: CORRELATED SINGLE TRACKS
MODEL 3: UNCORRELATED MULTIPLE TRACKS




**Example of GISAXS analysis using the MODEL UNCORRELATED MULTIPLE TRACKS.** (a) the ordering of the islands formed along the ion tracks, (b) AFM image of the irradiated surface (c) experimentally measured GISAXS map and (d) its simulation.

## HOW TO USE *GisaxStudio?*

1. DOWNLOAD THE PROGRAM from the site http://homer.zpr.fer.hr/gisaxstudio
2. LOAD THE EXPERIMENTAL GISAXS MAP
3. ENTER THE WANTED ACTIVITY (VISUAL GUESS, FIT or BATCH FIT)
4. CHOOSE THE MODEL AND PARAMETERS
5. 5TART THE FIT OR SIMULATION




One of the windows of the program ***GisaxStudio*** showing the experimental and simulated GISAXS maps. The parameters obtained by fit or used for the simulation appear below the images

## CONCLUSION

***GisaxStudio* is modular, multi-platform program written in Java programming language, featuring graphical user interface, built-in optimization algorithms and visualization. It is distributed in binary form (jar) and the installation process consists of unzipping the file. *GisaxStudio* runs on all major platforms (Linux, Windows and MacOS) provided that Java 1.8+ environment is installed. *GisaxStudio* stores all data in the relational database which facilitates data exchange and reproducibility. It was designed to be generic tool for various GISAXS models optimization, so that it can be easily extended with additional models and optimization algorithms. Our intent was to provide a computer aided GISAXS analysis tool that will be easy to use, extend, and will automatize various tedious tasks such as image preprocessing, raster areas definition, batch simulations, etc.**

## REFERENCES

[1] M. Buljan, N. Radić, S. Bernstorff, G. Dražić, I. Bogdanović-Radović, and V. Holý; "*Grazing incidence small angle x-ray scattering: application in study of quantum dot lattices*", Acta Cryst. A, 68, 124, (2012)
[2] M. Buljan, M. Karlušić et al. *GISAXS analysis of ion beam modified films and surfaces*. In preparation
[3] I. Mekterović et al. *GisaxStudio - a software platform for GISAXS analysis*. In preparation.

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