

NEW METHOD AND PROGRAM FOR GISAXS ANALYSIS OF ION-BEAM MODIFIED MATERIALS

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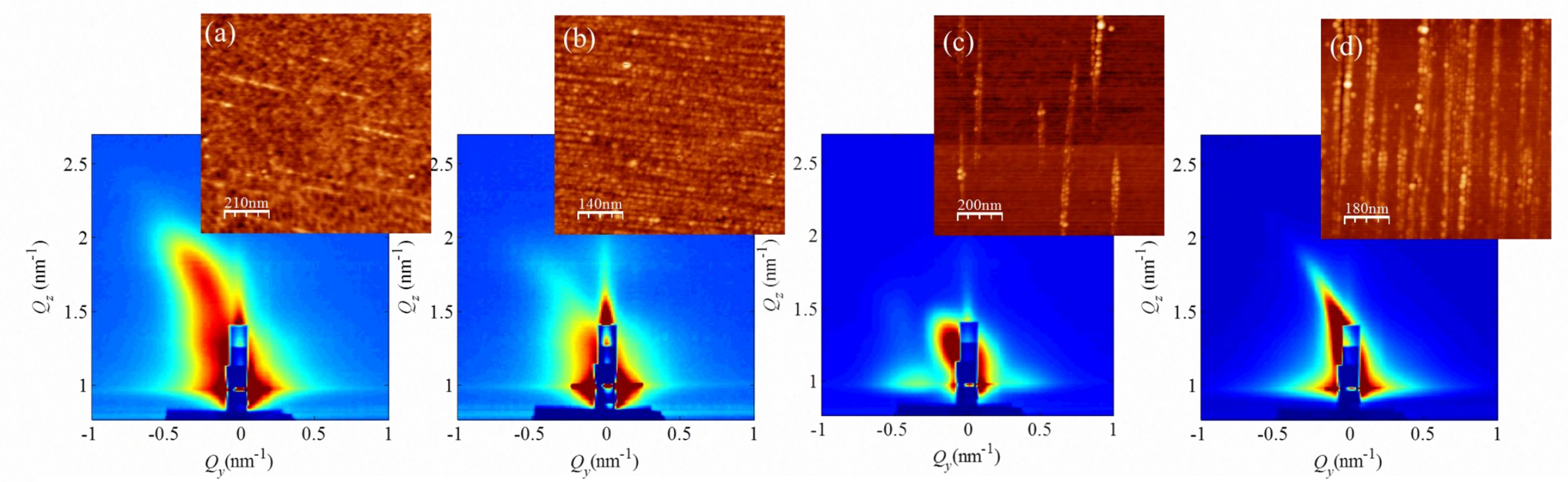
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INTRODUCTION

We present a method for the structural analysis of ion beam modified materials and their surfaces by GISAXS (grazing incidence small angle x-ray scattering). Several models describing different arrangement types of the nano-objects formed along ion-tracks are developed. They enable the determination of the structure and arrangement of the formed nano-objects including their mean structure, shape, size, separation and number of objects along the track, as well as their statistical distributions. The developed models are incorporated in a new software platform *GisaxStudio-iBeam*. It is a modular, multi-platform program written in Java programming language, featuring a graphical user interface, built-in optimization algorithms and visualization. It stores all data in the relational database which facilitates data exchange and reproducibility. It is free for non-commercial use and can be downloaded from the <http://homer.zpr.fer.hr/gisaxstudio>

SURFACE TRACKS- STRUCTURAL OVERVIEW:



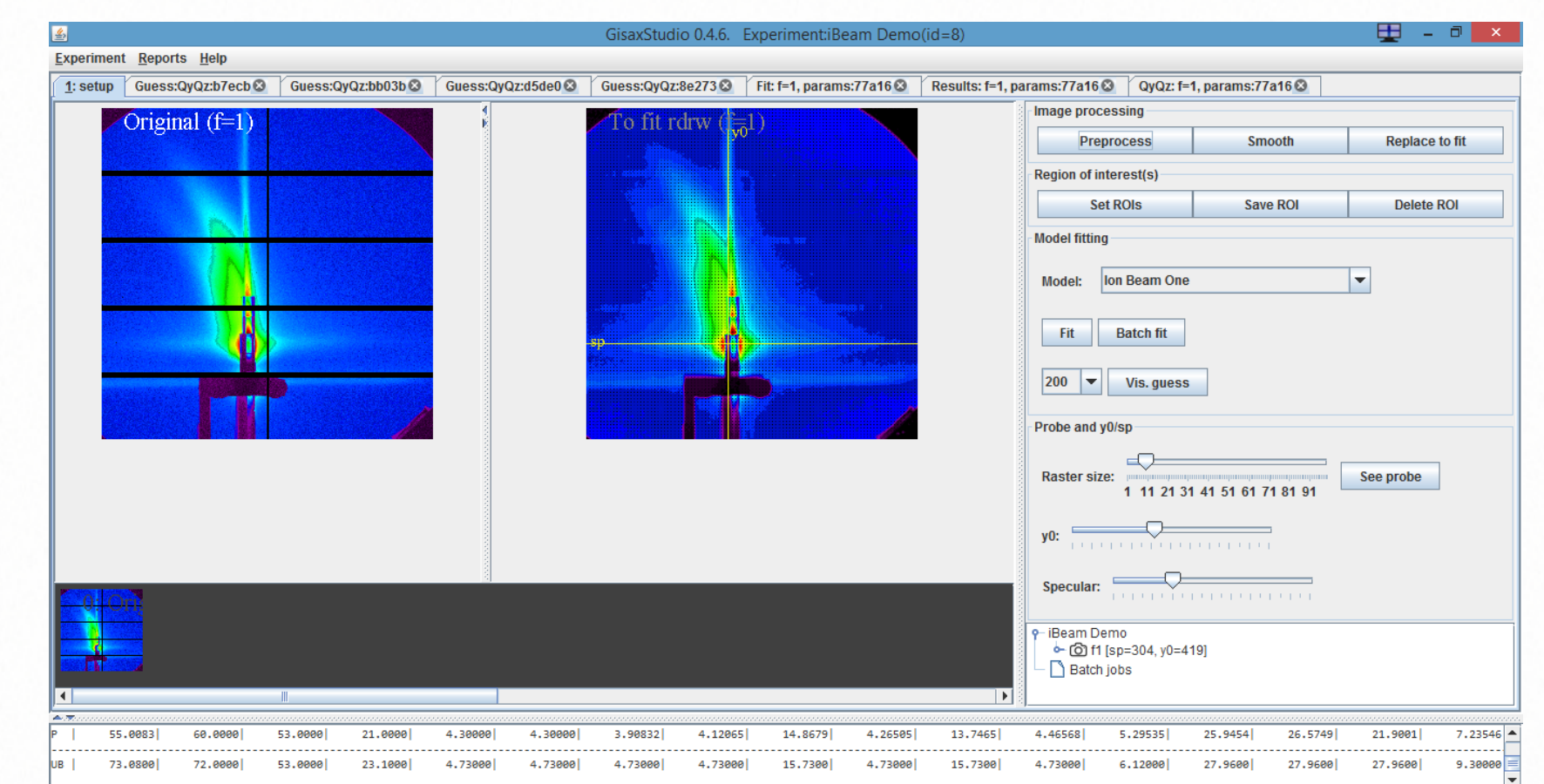
Surface tracks: examples showing different structural properties. GISAXS intensity distributions and corresponding AFM images (insets) measured on Ge+ITO films irradiated with different ion types and doses under angle of 1 deg. **A suitable theory is needed for the description of the GISAXS data.**

SOFTWARE PACKAGE *GisaxStudio-iBeam*:



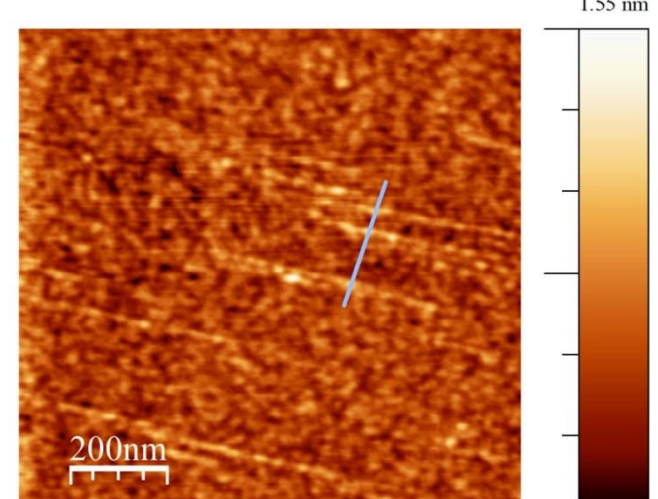
Software package *GisaxStudio* contains two families of models: - *3dLattice* for the analysis of three-dimensional quantum dot lattices formed by different self-assembly processes and *-iBeam* which is suitable for the analysis of GISAXS intensity distributions measured on ion-beam modified materials.

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



Main window of *GisaxStudio-iBeamM*

MODEL 1: ISOLATED TRACKS



This model describes surface tracks consisting of islands making 2D lattice described by basis vectors: a_1 (SRO, LRO) and a_2 (R,R). * This model is suitable for the description of surface tracks formed by low-dose irradiation. * The terms in brackets refer to the ordering type of the x and y components of the basis vectors [1].

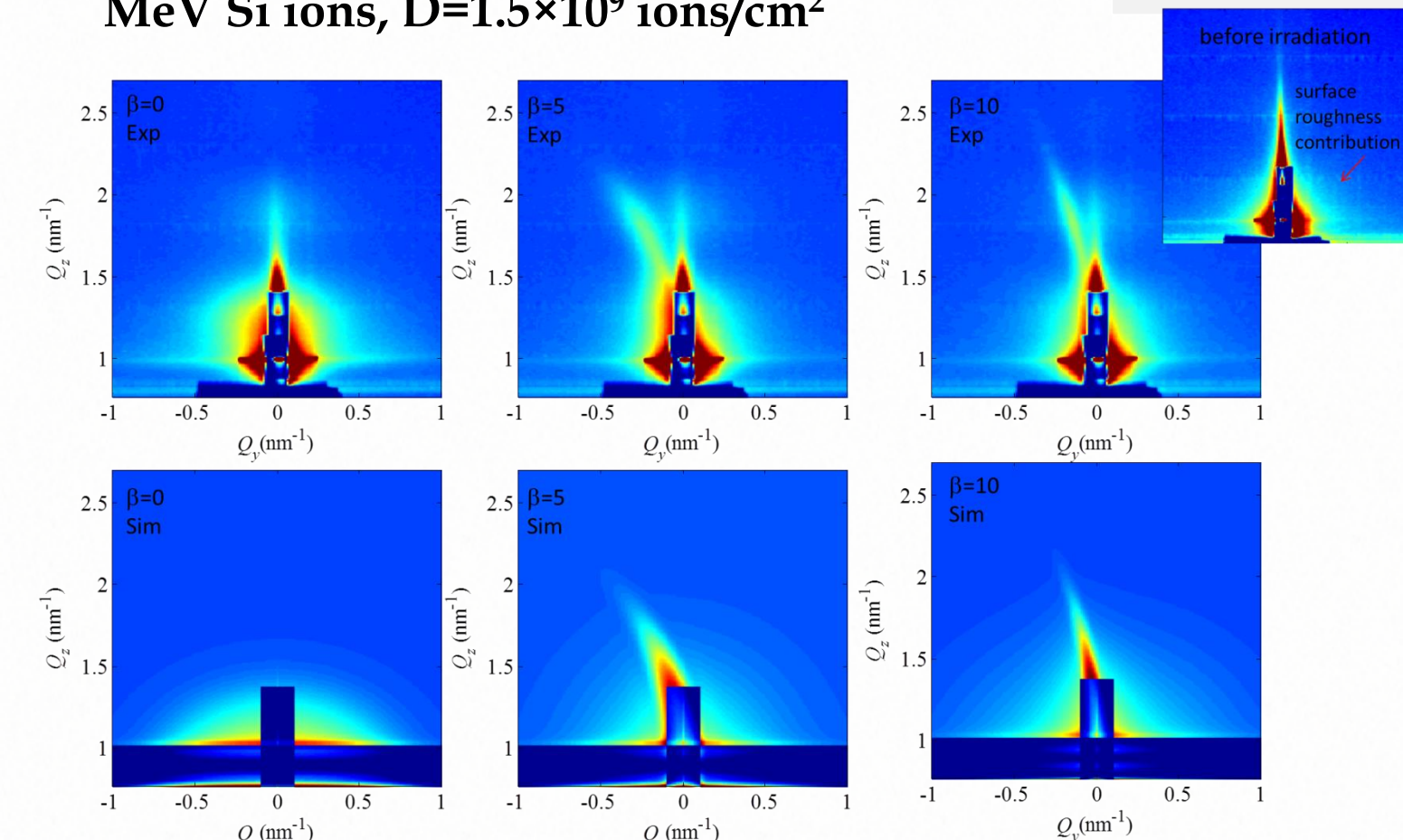
PARAMETERS (AFM):

$R_z = 0.8 \pm 0.2$ nm
 $|a_1| = 25 \pm 8$ nm
 $N_i = 20 \pm 10$

PARAMETERS (GISAXS):

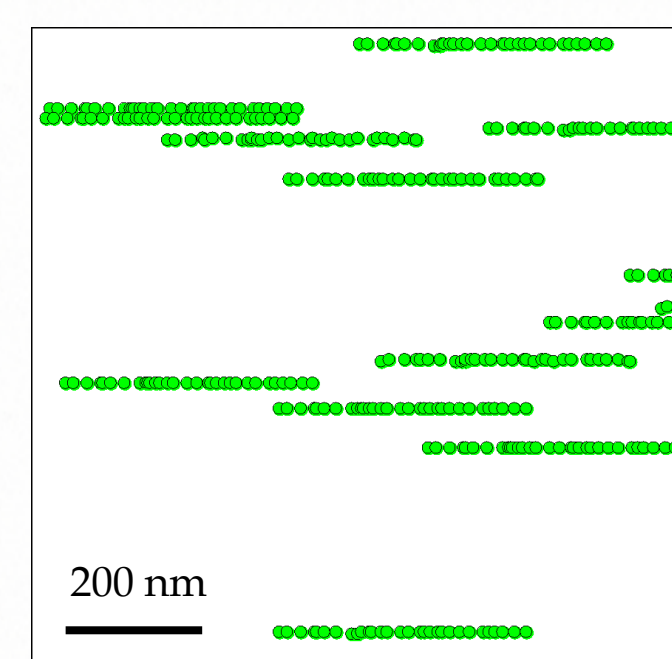
$R_x = R_y = 2.1 \pm 0.2$ nm
 $R_z = 1.0 \pm 0.1$ nm
 $|a_1| = 20 \pm 2$ nm
 $N_i = 32$
 $\sigma_{1x} = 10 \pm 2$ nm
 $\sigma_{1y} = 0.2 \pm 0.1$ nm

Isolated tracks: AFM image of Ge+ITO surface irradiated with 15 MeV Si ions, $D = 1.5 \times 10^9$ ions/cm²

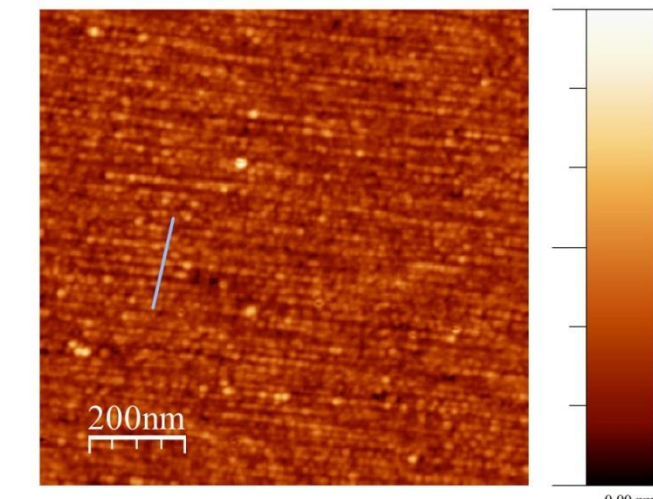


Example of application of Model 1: GISAXS maps of Ge+ITO surface irradiated with 15 MeV Si ions, $D = 1.5 \times 10^9$ ions/cm², $\phi_{irr} = 1$ deg. Different angles (β) between probing x-ray beam and irradiation direction are shown.

Simulation of the island positions. The positions are obtained using the parameters of the GISAXS fit.



MODEL 2: CORRELATED TRACKS



This model describes surface tracks consisting of islands making 3D lattice on the surface described by basis vectors a_1 (SRO, LRO), a_2 (R,SRO) and a_3 (SRO, LRO). This model is suitable for the description of surface tracks formed by high-dose irradiation (ion track overlapping) which causes correlation in separation between ion tracks.

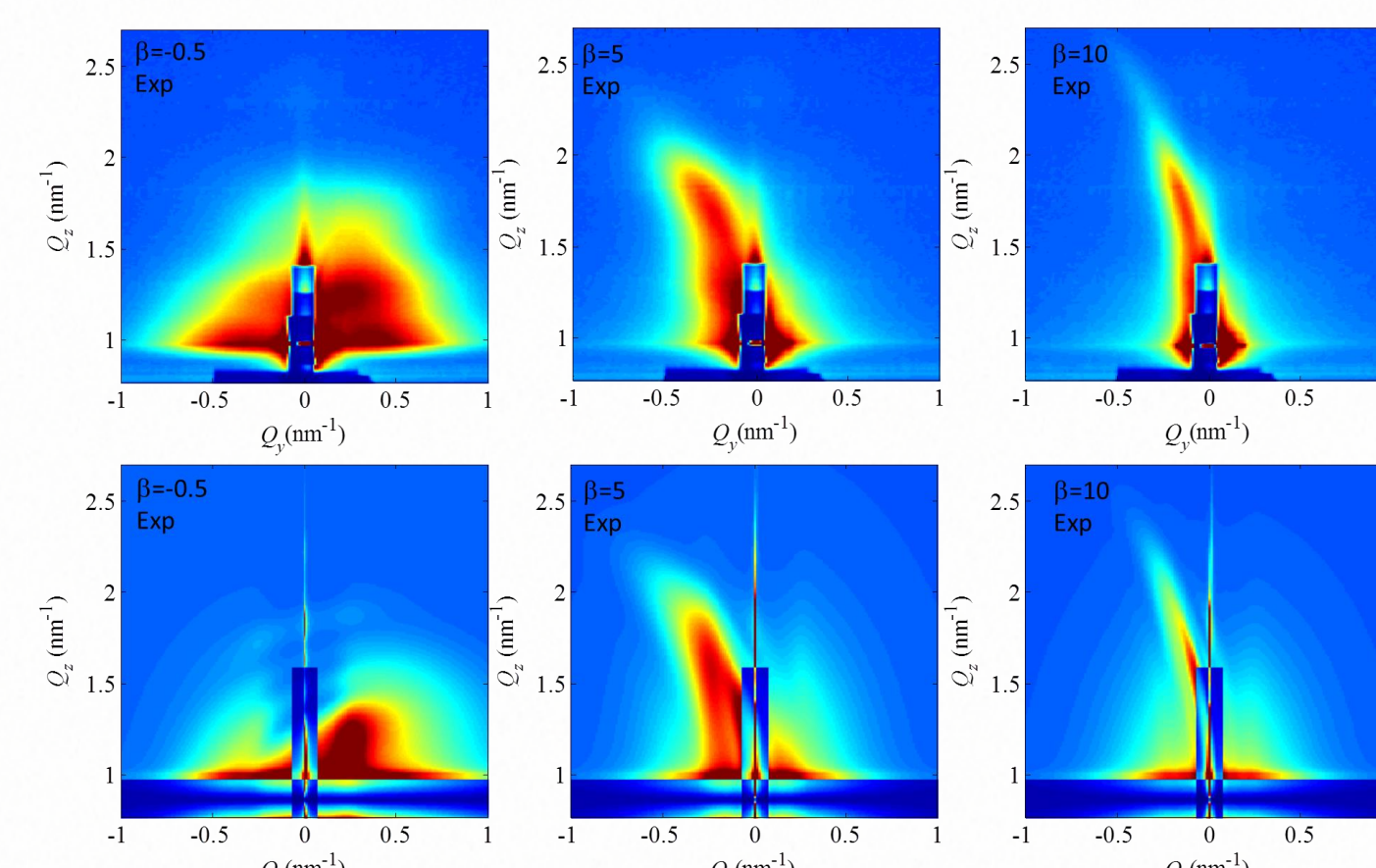
PARAMETERS (AFM):

$R_x = 1.1 \pm 0.2$ nm
 $|a_1| = 18 \pm 3$ nm
 $|a_2| = 18 \pm 4$ nm
 $N_i = 15 \pm 5$

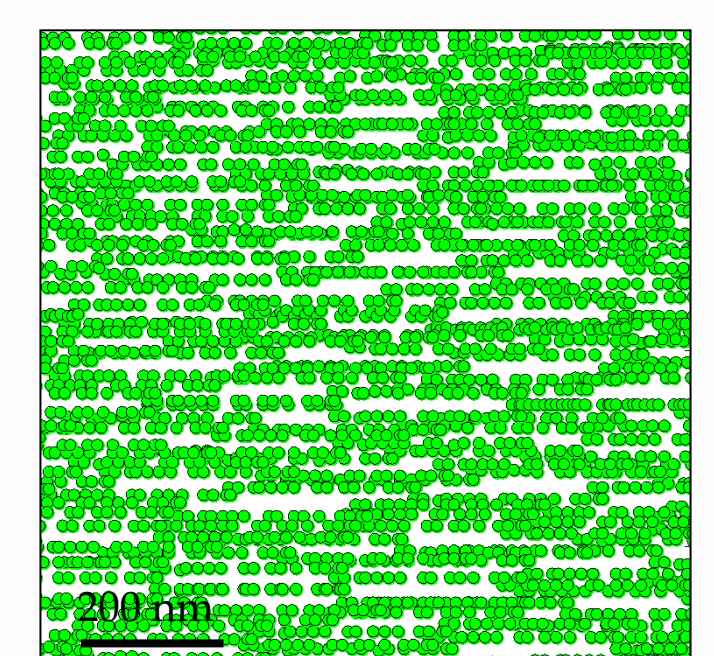
PARAMETERS (GISAXS):

$R_x = 2.7 \pm 0.2$ nm
 $R_y = 2.7 \pm 0.2$ nm
 $R_z = 1.3 \pm 0.1$ nm
 $|a_1| = 17 \pm 1$ nm
 $|a_2| = 18.5 \pm 0.7$ nm
 $N_i = 15$
 $\sigma_{1x} = 7 \pm 1$ nm
 $\sigma_{1y} = 0.2 \pm 0.2$ nm
 $\sigma_{2y} = 3.9 \pm 0.5$ nm
 $\sigma_{3x} = 13 \pm 5$ nm
 $\sigma_{3y} = 5 \pm 2$ nm

Correlated tracks: AFM image of Ge+ITO surface irradiated with 15 MeV Si ions, $D = 2.5 \times 10^{10}$ ions/cm²

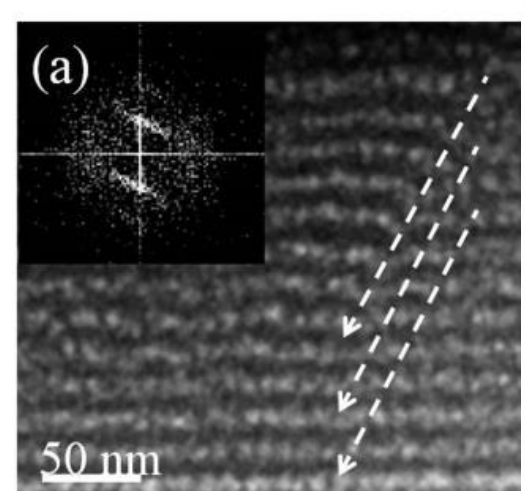


Example of application of Model 2: GISAXS maps of Ge+ITO surface irradiated with 15 MeV Si ions, $D = 2.5 \times 10^{10}$ ions/cm², $\phi_{irr} = 1$ deg. Different angles (β) between probing x-ray beam and irradiation direction are shown.



Simulation of the island positions. The positions are obtained using the parameters of the GISAXS fit.

MODEL 3: TRACKS IN MULTILAYER FILMS



This model describes ion tracks consisting of QDs making 3D lattice in a 3D (multilayer) film described by basis vectors $a_1 = a_2 = (SRO, SRO, LRO)$, and $a_3 = (SRO, SRO, LRO)$. This model is suitable for the description of quantum dots or islands formed by irradiation under larger incidence angles or correlation of QDs formed by plastic deformation caused by ion beam.

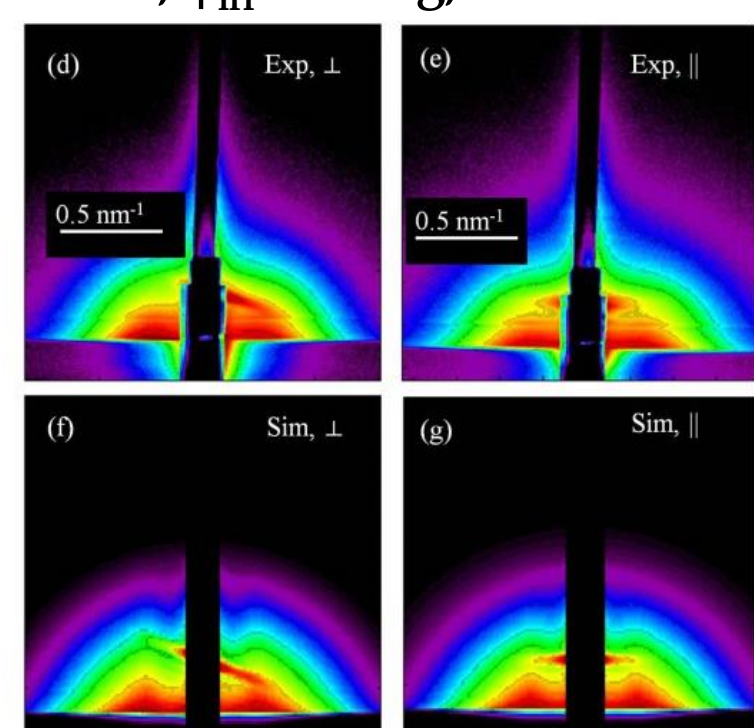
PARAMETERS (TEM):

$R_x = 4.1 \pm 0.5$ nm
 $R_z = 4.1 \pm 0.25$ nm
 $|a_1| = 21 \pm 4$ nm
 $|c| = 14 \pm 1$ nm
 $N_i = 20$

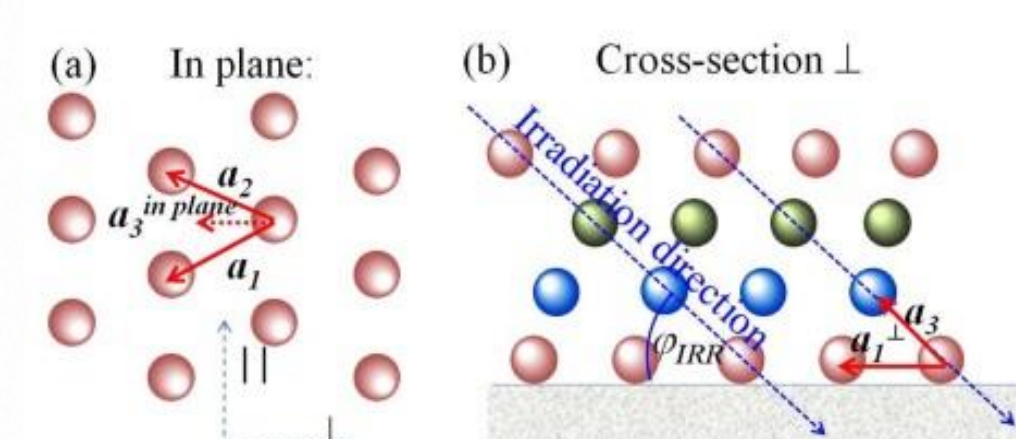
PARAMETERS (GISAXS):

$R_x = R_y = 4.1 \pm 0.1$ nm
 $R_z = 4.1 \pm 0.1$ nm
 $|a_1| = 21.0 \pm 1$ nm
 $|c| = 14.6 \pm 0.7$ nm
 $N_i = 20$
 $\sigma_{1x,y} = \sigma_{2x,y} = 8.6 \pm 0.4$ nm
 $\sigma_{3x,y} = 8.0 \pm 50.2$ nm
 $\sigma_{3z} = 1.1 \pm 0.2$ nm

Tracks in multilayer: TEM image of Ge+SiO₂ irradiated film with 16 MeV O ions, $\phi_{irr} = 60$ deg, $D = 1 \times 10^{15}$ ions/cm²



Example of application of Model 3 irradiation with 10 MeV O ions, $D = 1 \times 10^{15}$ ions/cm². Two different angles ($\beta = 0$, and 90 deg) between probing x-ray beam and irradiation direction are shown.



Model of the observed QD ordering. (a) ordering within each layer, (b) ordering in different layers.

CONCLUSION

We have developed theoretical models for the description of GISAXS intensity distributions from various types of discontinuous surface tracks formed by ion beam irradiation. The track types differ by the ordering of nano-islands formed by irradiation and by the disorder degree. The models are supported with experimental examples showing applications of the models on real systems. The structural parameters obtained by the GISAXS analysis using the developed models are in a good agreement with the parameters obtained from atomic force microscopy. The developed models can be applied to a wide variety of systems and they enable for a precise determination of the island ordering type, its parameters, disorder type and degree of disorder, as well as island size and size distribution. The details of the models will be published in Ref. [2]. The models are incorporated in software package *GisaxStudio-iBeam* [3].

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 irradiated films and surfaces. In preparation
- [3] I. Mekterović, D. Mekterović, S. Bernstorff and M. Buljan, *GisaxStudio - a software platform for GISAXS analysis*. In preparation.

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