

Introduction to DeepDWBA

G. Pospelov, D. Yurov, **M. Ganeva**

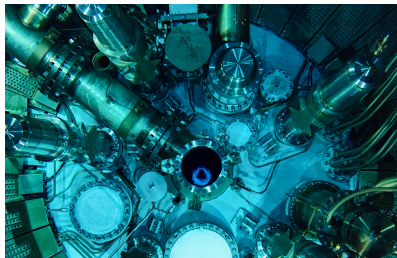
JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

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MLZ is a cooperation between

DeepDWBA team

works in Scientific Computing Group of Heinz Maier-Leibnitz Zentrum (MLZ)



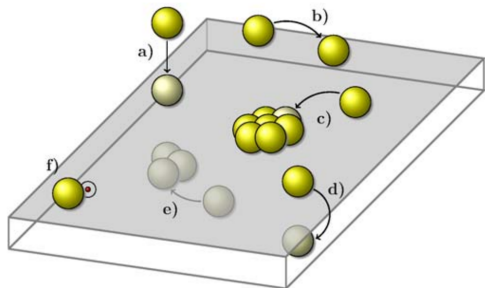
Neutron and X-ray scattering data analysis:

reciprocal space \rightarrow real space

only amplitude is measured, phase is unknown

Thin film growth from atomic deposition

multiple processes simultaneously



- a deposition of atoms
- b surface diffusion
- c cluster growth
- d diffusion into the bulk
- e diffusion and cluster growth in the bulk
- f trapping at defect sites

Rosenthal et. al., 2011,
doi:10.1002/ctpp.201100034

growth mechanism \iff **film morphology** \implies **film properties**

Grazing-incidence small-angle scattering

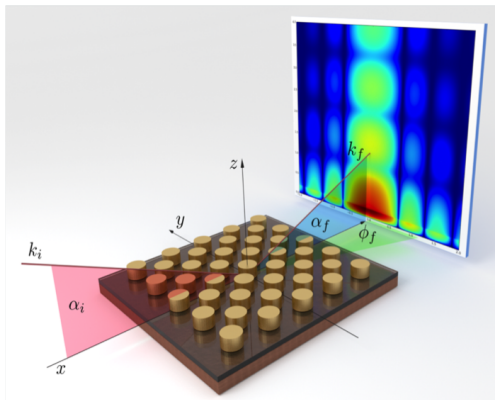
morphological characterization technique in reciprocal space

Suitable to probe

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

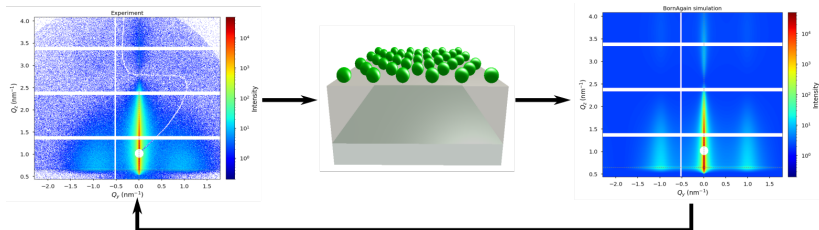
Benefits

- 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

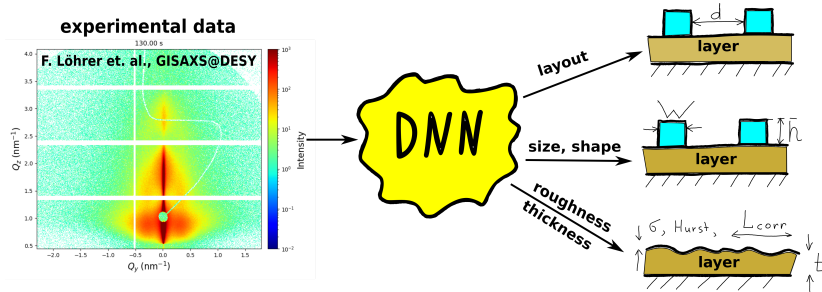


- Reciprocal space, phase information is lost
- Multiple reflections at interfaces due to small incident angle.
- Simulation required for each step \Rightarrow time-consuming
- High dimensional vector of fit parameters

$10^4 - 10^5$ images per synchrotron experiment

DeepDWBA: plans for hackathon

train the neural network on synthetic data; apply to experimental data



Expected result:

- fast feedback on thin film morphology
- understanding of film growth mechanism

Thank you
for your attention!

