Deep learning for small angle scattering under grazing incidence

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Grazing-incidence small-angle scattering

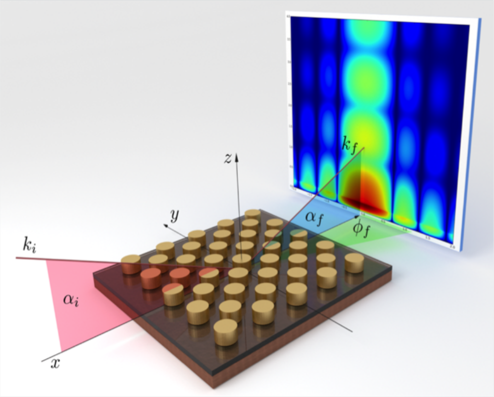
morphological characterization technique in reciprocal space

Suitable to probe

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

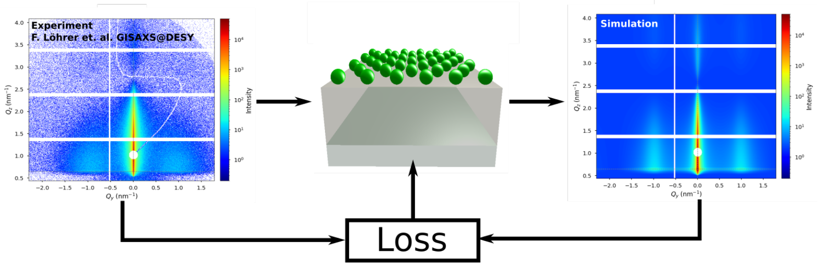
Benefits

- 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



- Multiple reflections at interfaces due to small incident angle.
- Simulation required for each step $\Rightarrow$ time-consuming
- High dimensional vector of fit parameters

some data is impossible to fit!

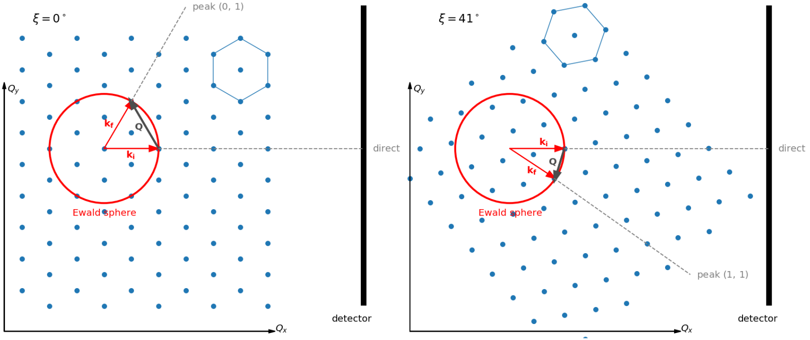
Challenge 1

Walter Van Herck, Jonathan Fisher, Marina Ganeva

Predict orientational distributions
for hexagonally arranged nanoparticles

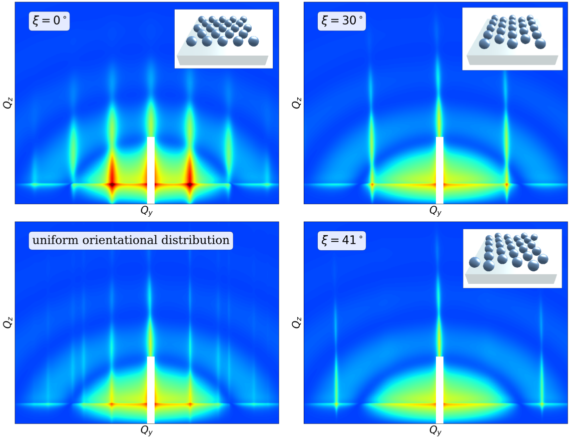
GISAS on hexagonally arranged nanoparticles

Lattice rotation in reciprocal space



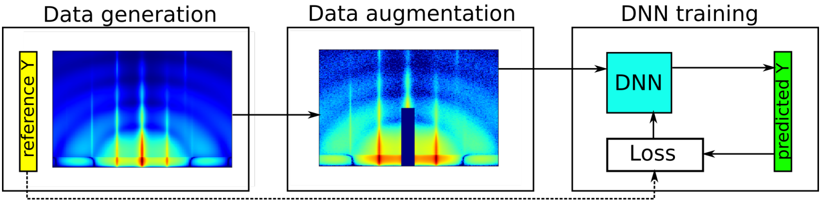
peak is observed only if the Ewald sphere intersects a lattice point

GISAS on hexagonally arranged nanoparticles



- Multiple domains with different orientations
- Orientational distribution is impossible to fit!

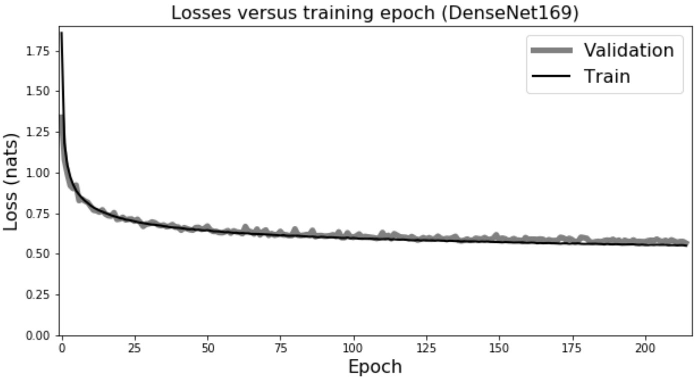
Solution: train deep neural network



Concerns	Solutions
no labeled experimental data	use simulated data
overfitting	variable simulation parameters data augmentation large amount of data (500K)
evaluation	validation data (simulated)

Chosen architecture: DenseNet169 (12.8M of parameters)

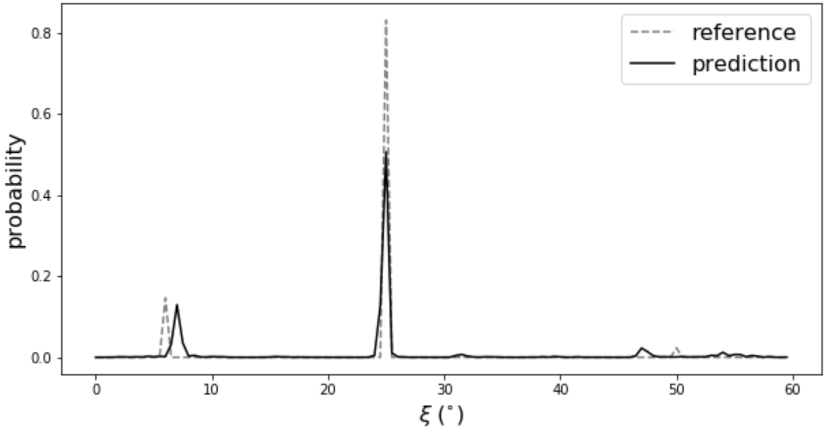
Model evaluation: learning curve



no overfitting, no exploding gradients

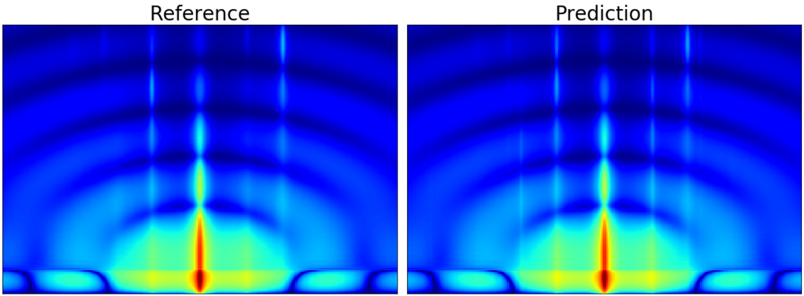
Prediction for validation data

Compare orientational distributions



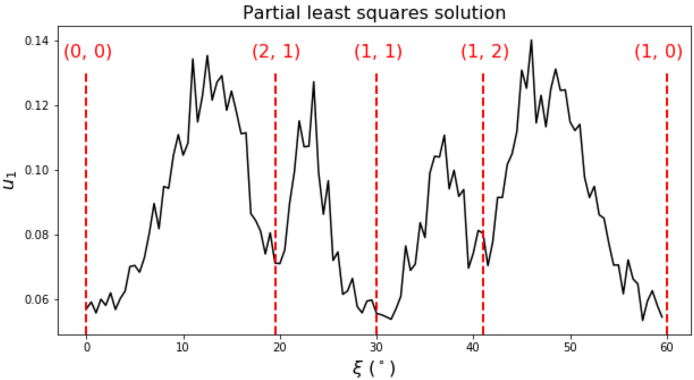
Prediction for validation data

Compare simulated GISAS patterns



GISAS patterns look very similar

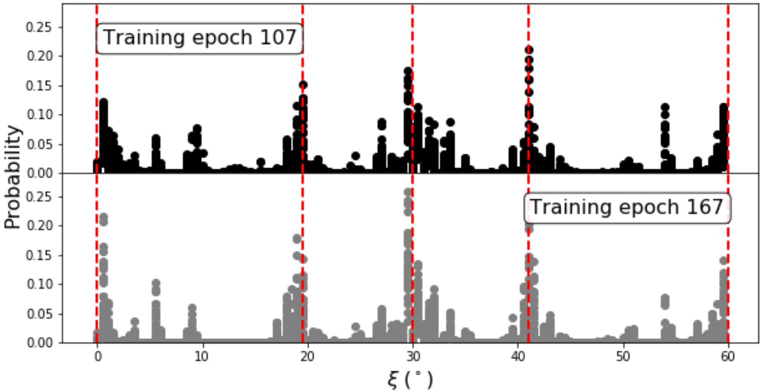
Partial least squares analysis



peaks: difficult to predict
valleys: easier to predict

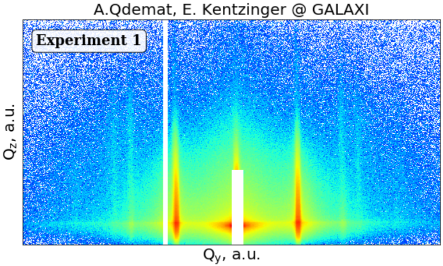
Analysis of possible bias

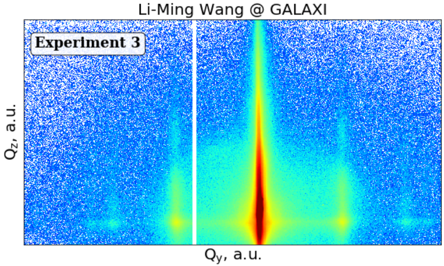
Prediction for uniform input orientational distribution



Prediction is noisy, but tends to 5 angles

Prediction for experimental data [1,2]





Expert scientist guess:

two angles of lattice rotation: $xi = 0^\circ$ and $xi = 30^\circ$

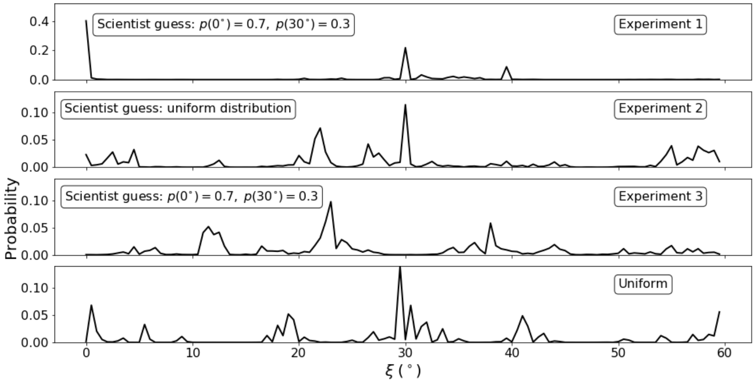
probabilities: $p(0^\circ) = 0.7,\ p(30^\circ) = 0.3$

[1] Asmaa Qdemat, PhD Thesis (to be submitted)

[2] Li-Ming Wang, PhD Thesis (2018)

Prediction for experimental data

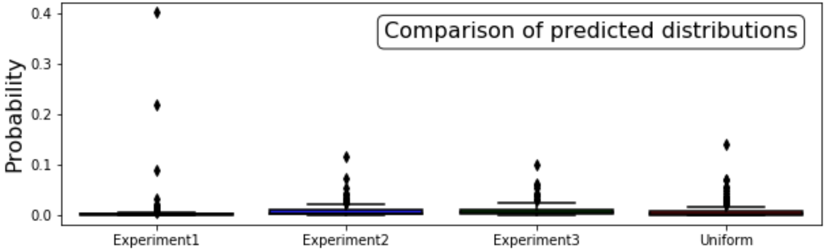
Comparison of predicted distributions



predictions for Experiments 2 and 3 similar to one for uniform

Prediction for experimental data

Properties of predicted distributions

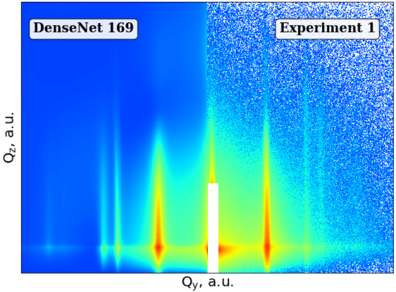


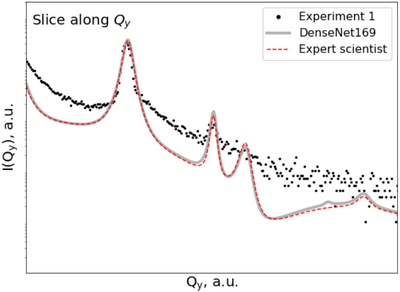
Simple statistical analysis

- confirms hypothesis about similarity of distributions predicted for experiments 2 and 3 to one predicted for uniform
- rejects this hypothesis for experiment 1

$\Rightarrow$ **Experiments 2 and 3 have uniform rotational distribution**

Prediction for experimental data: Experiment1



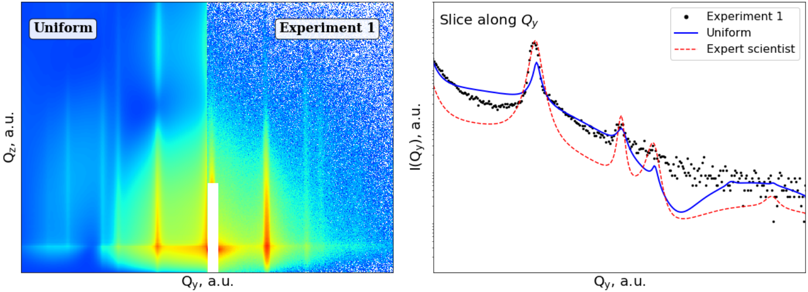


+ peak positions and relative intensities match well
− diffuse scattering is not fully reproduced

would uniform distribution perform better?

Prediction for experimental data: Experiment1

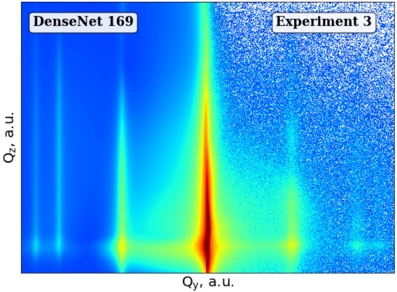
DenseNet prediction vs. uniform distribution

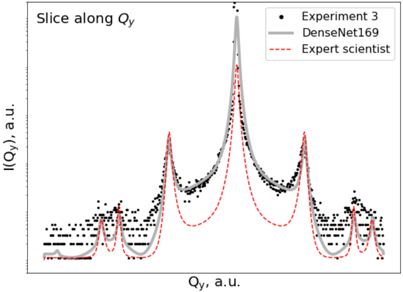


- relative intensities do not match
- diffuse scattering is overestimated

$\Rightarrow$ **DenseNet prediction performs better, than uniform**

Prediction for experimental data: Experiment3



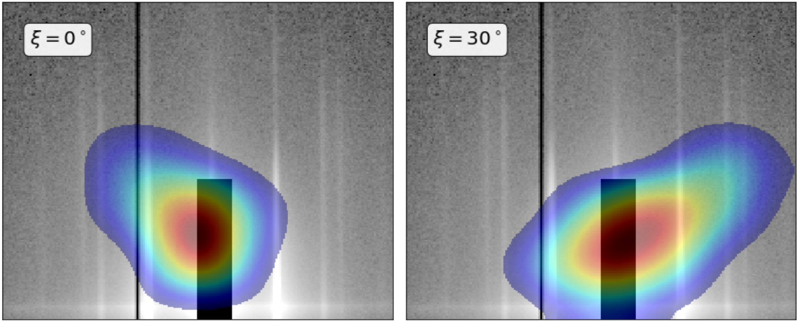


+ peak positions and relative intensities match well
+ DenseNet prediction better reproduces diffuse scattering

DenseNet gives better prediction!

What contributes to prediction?

Attention maps[3] for Experiment 1



DenseNet pays attention to peaks!

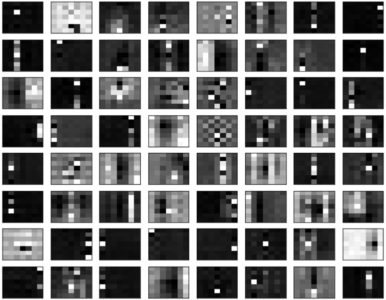
[3] Attention maps created with *keras-vis* library: R. Kotikalapudi et. al., 2017, https://github.com/raghakot/keras-vis

Learning transfer: could we benefit?

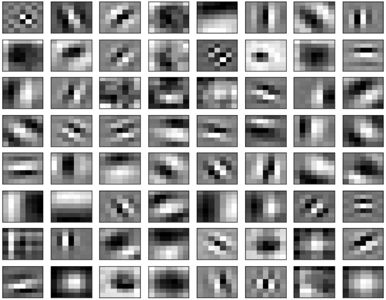
Cartoon: https://medium.com/free-code-camp/asl-recognition-using-transfer-learning-918ba054c004

DenseNet 169 conv0 filters

Trained on GISAS data



Trained on ImageNet



Network learns different basic features

Challenge 2

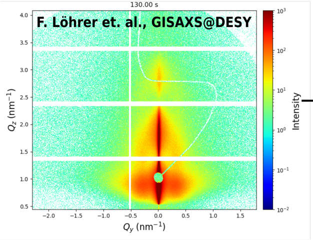
G. Pospelov, D. Yurov, N. Hoffmann, M. Ganeva

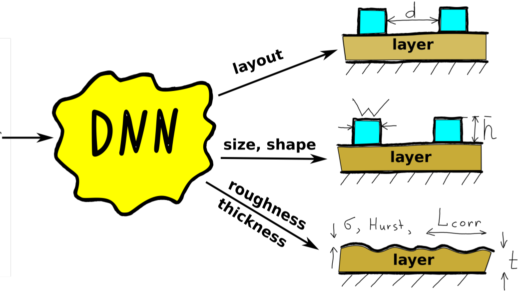
Predict sample parameters for GISAS pattern

GISAS study of thin film growth

New: started in September 2019

experimental data



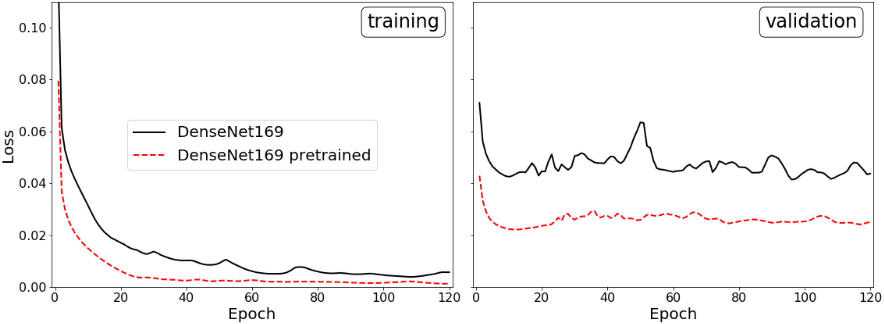


For understanding of film growth mechanism:

+ $10^4 - 10^5$ **GISAXS patterns per experiment**
- **experimental data are not labeled**
! **fast feedback on thin film morphology needed**

Learning transfer: could we benefit?

Experiments done at cluster of TU Dresden



Loss for pretrained network is smaller and decreases faster!

To be continued..

Conclusion

Deep learning for GISAS

Challenge 1: predict orientational distribution

+ DenseNet 169 makes predictions with reasonable performance
+ Model trained with artificial data works also for experimental GISAS patterns

! We need more experimental data from different instruments to test the model

Challenge 2: extract thin film parameters

- Loss for pretrained networks decreases faster and is lower
- The work is in progress

DNN makes prediction in microseconds

Acknowledgments

Data provided for model testing:

- A. Qdemat, E.Kentzinger (Experiments 1 and 2)
- L.-M. Wang (Experiment 3)
- F. Löhrer (film growth)

Access to GPU cluster:

- TU Dresden
- Organizers of Dresden Deep Learning hackathon

All simulations have been done with

BornAgain (bornagainproject.org)

Thank you for your attention!