Remote PACBED Thickness Determination by CNNs

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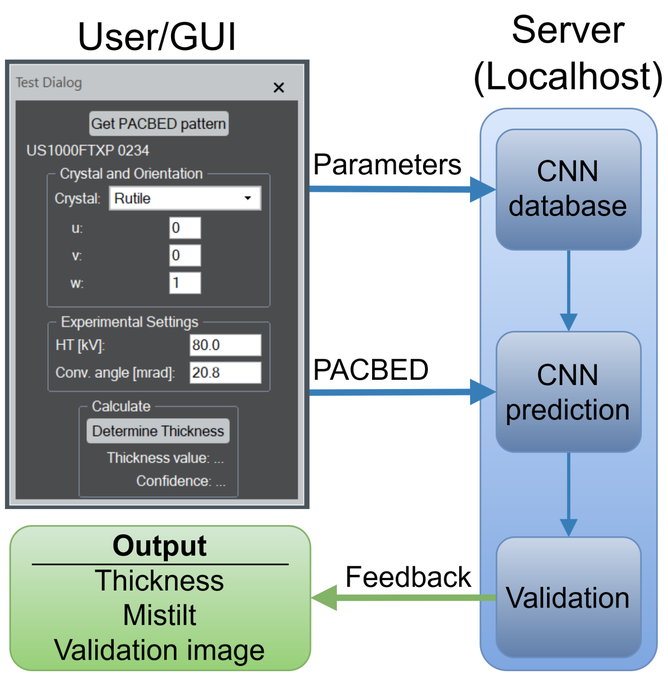
Introduction

A convenient thickness determination technique for crystalline samples is the position averaged convergent-beam electron diffraction (PACBED) method [1]. The thickness is determined by finding the best match of the recorded PACBED pattern with a series of simulated PACBEDs. This process can be automatized by convolutional neural networks (CNNs), making the method fast and easy to apply [2]. However, the simulation of a synthetic dataset and the training of the CNNs have high computational cost and these CNNs are only valid for the specific trained system. Therefore, we built a working prototype of a server-based thickness determination by CNNs with a shared CNN-database and a GUI. By this, every scientist, even without knowledge about machine learning and multislice simulation, could determine the specimen thickness by PACBEDs within few seconds during a microscope session.

Prototype



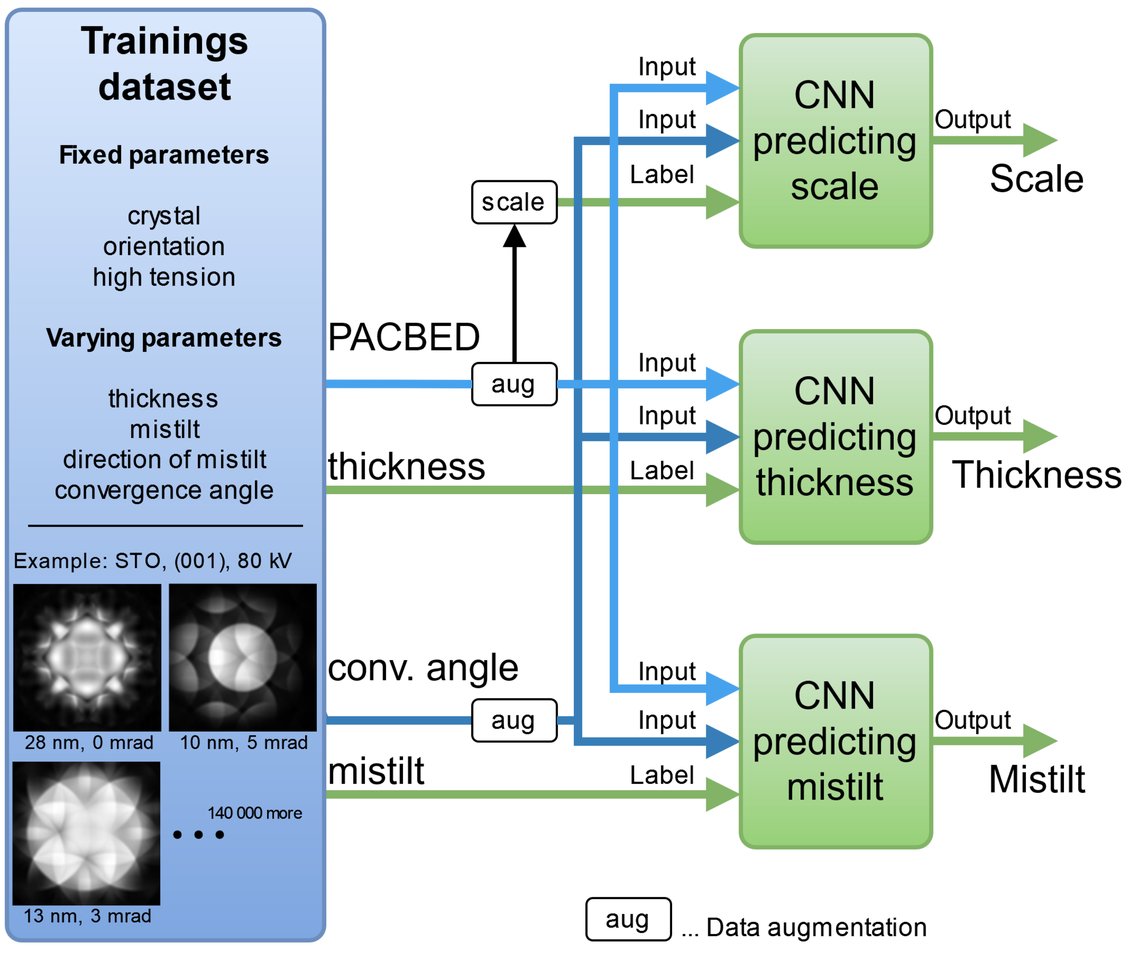
GUI/User:
- Select PACBED
- Enter parameters
- Upload data

Server:
- Selecting correct CNNs
- Pre-processing PACBED
- Making prediction
- Generating feedback

User:
- Verify results

Convolutional Neural Networks

The PACBED analysis is performed by three different trained CNNs (scale, thickness and mistilt). The synthetic trainings dataset is generated by multislice simulations. The system is only valid for the fixed parameters and within the range of the varying parameters.



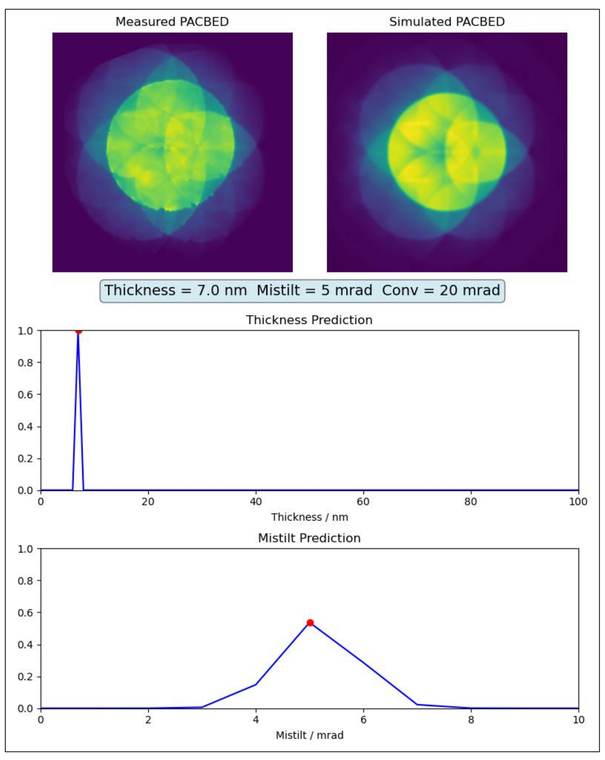
Results

Due to possible misclassification of CNNs, the prediction should be verified by comparing the images in the validation image. Misclassification can be caused by wrong given input parameters or bad quality of the recorded PACBED.

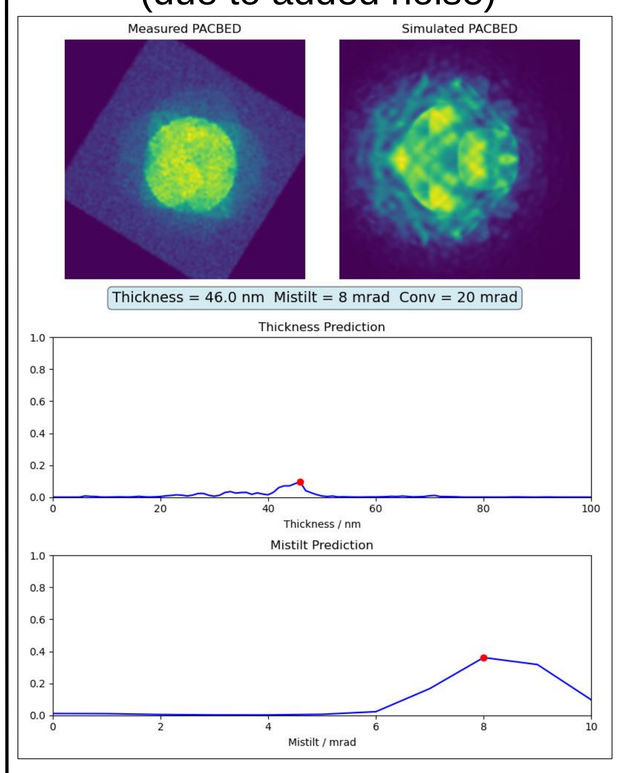
Example

Rutile in [001]-direction at 80kV and 20 mrad conv. angle

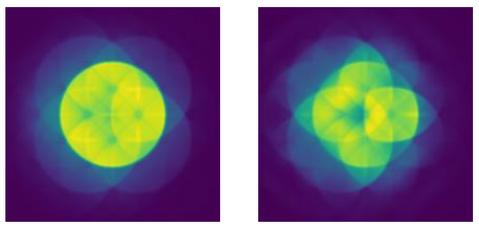
Correct classification



Misclassification
(due to added noise)

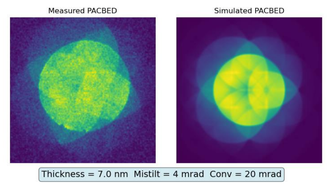


PACBEDs close to the predicted thickness



5 nm 9 nm

Misclassifications are easy to identify by the validation image.



→ Correct prediction

CNNs are robust against noise.

Summary & Outlook

The feasibility of the remote PACBED thickness determination concept has been proven with two different material systems (TiO_2 and STO). In future, the published version will have a automatic pipeline (simulation and training of CNNs) for requested non-available material systems.

References/ Literature

[1]J. M. LeBeau, S. D. Findlay, L. J. Allen, and S. Stemmer, Ultramicroscopy, vol. 110, no. 2 (2010)
[2]W. Xu and J. M. LeBeau, Ultramicroscopy, vol. 188 (2018)

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