Machine Learning in Coherent Fourier Scatterometry for the distinction of geometric structures of spherical gold nanoparticles

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A machine learning model that distinguishes geometric arrangements of nanoparticles based on measurements within the Fourier plane with Coherent Fourier Scatterometry is presented. An existing using learning model was succesfully retrained using a custom dataset genereated from our mesurement data.

1 Introduction

Coherent Fourier Scatterometry (CFS) is an easy-to-implement far-field optical method. This method could be used in the semiconductor industry to detect systematic process errors, i.e. direction-dependent defects or contamination, more quickly. Our CFS analysis evaluates the diffraction spectrum in the Fourier plane of a high numerical aperture (NA) microscope objective [1]. In a more detailed work, it has already been shown that different geometric arrangements of nanoparticles can be distinguished from each other by taking the Fourier transform of the measured pupil image [2]. We now show the next logical step towards an automated application of this method by training a machine-learning model that can autonomously distinguish the measurement data. To demonstrate the general feasibility, an existing model is selected and trained with our specific data.

2 Methods

In this work, the classification of 6 different geometries (classes) of nanoparticle arrangements is analyzed. The CFS measurements processed in the form of Fourier transformations with their corresponding particle geometries are shown in *Figure 1*. A detailed description of the sample preparation process and the CFS measurements can be found in [2]. The two-dimensional Fourier transformations of the pupil images, that can be interpreted as aberrated Point Spred Functions (PSFs), allow a clear differentiation of the measured assemblies.
A machine learning approach is used to investigate wheter it is possible to train a model to distinguish the different geometries. Since we only have one structure per (Fourier transformed) pupil image that needs to be classified, we need a single object detection algorithm. Detectron2 is a software system that implements state-of-the-art object detection algorithms [4]. It is built using PyTorch and offers a variety of pre-trained models. The COCO-Detection/retinanet_R_101-algorithm from the Detectron2 model zoo is suitable for our application since it is tasked with localizing the objects present in an image, and at the same time, classifying them into different categories [3]. It is a popular single-stage detector, which is accurate and runs fast. This gives us an easy-to-implement tool.

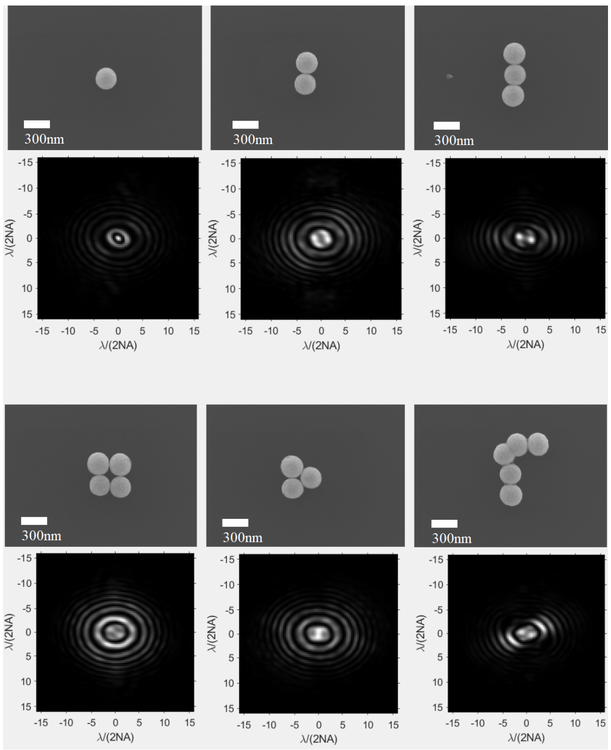

Fig. 1 *The geometries to be distinguished with the corresponding CFS measurement signals which are processed using a Fourier transformation.*

Our custom dataset consists of 171 images, 70% of which are used for retraining the existing model, 20% for validation and 10% are retained for testing afterwards. The YOLO ('You Only Look Once') data format is used for the annotations and the bounding box is defined around the first four rings of the aberrated PSF from each Fourier transformed image. Each particle geometry (1x1, 2x1, 3x1, 2x2, triangle and L-shape) corresponds to a class (0,1,2,3,4,5) and is noted in the annotation. For the training pro-

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cess a learning rate of 0.00025 and 6000 iterations are used. The current status of the model is saved as a checkpoint every 500 iterations. After training, the learning performance of the model is evaluated and the best model is selected from the various temporarily stored models. This model is then used to predict the classes of the unknown test images.

3 Results

After the training has been completed, the model must first be validated. For this purpose, we plot the loss functions in dependence of the iterations. The goal is to find a well-trained, but not overtrained model. *Figure 2* visualizes the training and validation loss. The training loss indicates how well the model is fitting the training data, while the validation loss indicates how well the model fits new data.

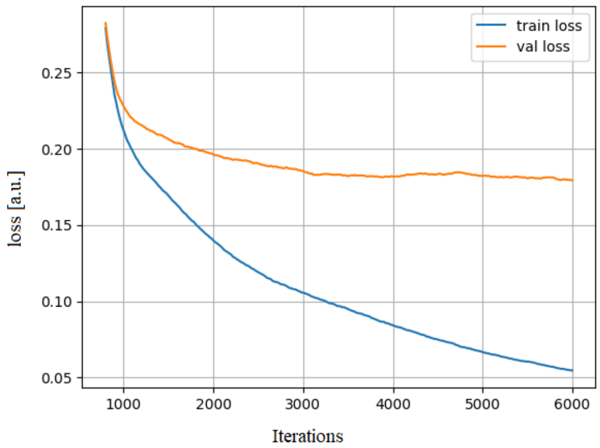

Fig. 2 *Plot of the loss functions for the retraining of the machine learning model.*

A plateau for the validation loss is reached at around 3000 iterations. This means that no improvement will be achieved with further iterations. Therefore, we will choose the model saved as a checkpoint at 3000 iterations for our evaluations. For the predictions of the 17 unknown test images, we use the 'predict'-function built into Detectron2, where we select our chosen model from the 3000 iteration checkpoint and the image to be classified as input parameters. The output is not a label, but a probabilistic score. This score indicates the probability with which the object found is assigned to a specific class. The results for the predictions of the test images are shown in *Table 1*. It can be seen that the geometric arrangements, with the exception of the triangle, are correctly classified with over 92% accuracy. The deviation for the triangle class can be explained by the fact that the triangle had the least measurement data available for training the model. In order to assign the results to a class, a threshold of 0.5 was selected, which is common in machine learning. Each image has only had one score above 0.5. With this score the image was assigned to the correct class of the present particle geometry.

geometry	assigned class	accuracy
1x1	0	0,923 $\pm$ 0,043
2x1	1	0,979 $\pm$ 0,011
3x1	2	0,982 $\pm$ 0,003
2x2	3	0,993 $\pm$ 0,004
Triangle	4	0,826 $\pm$ 0,220
L	5	0,994 $\pm$ 0,003

Tab. 1 *Accuracy for the classification of the different sample geometries.*

This is an excellent result due to the fact that we did not even focus on optimizing the individual parameters and weights for the training environment, but only carried out a simple feasibility study. With further optimization, we should be able to achieve even better results. We have thus successfully demonstrated the ability to use machine learning for the automated classification of our CFS measurement data that we have obtained from different geometric arrangements of spherical nanoparticles.

4 Conclusion

In this work we have retrained a pre-trained machine learning model for the classification of Fourier-transformed CFS measurement data using Detectron2 with PyTorch. The retrained model assigns the measurement data of six different spatial arrangements of nanoparticles on a Si wafer to the correct geometries with high accuracy. The volume of the training data set contains only 171 images. For further development of the model this data set must be significantly extended by additional measurement data. In addition, the training parameters such as the number of iterations or learning rate should be optimized in order to achieve, among other things, that training and validation loss are closer together and that the model becomes better. Nevertheless, we were able to demonstrate very well the feasibility of using machine learning for this task.

References

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