Fraunhofer IISB

Fraunhofer Institute for Integrated Systems and Device Technology IISB

3D Mask Simulation and Lithographic Imaging using Physics-Informed Neural Networks (PINN)

Vlad Medvedev, Andreas Erdmann*, Andreas Rosskopf
Fraunhofer Institute for Integrated Systems and Device Technology (IISB), Erlangen, Germany

SPIE Advanced Lithography + Patterning 2024, San Jose, California, United States

Author

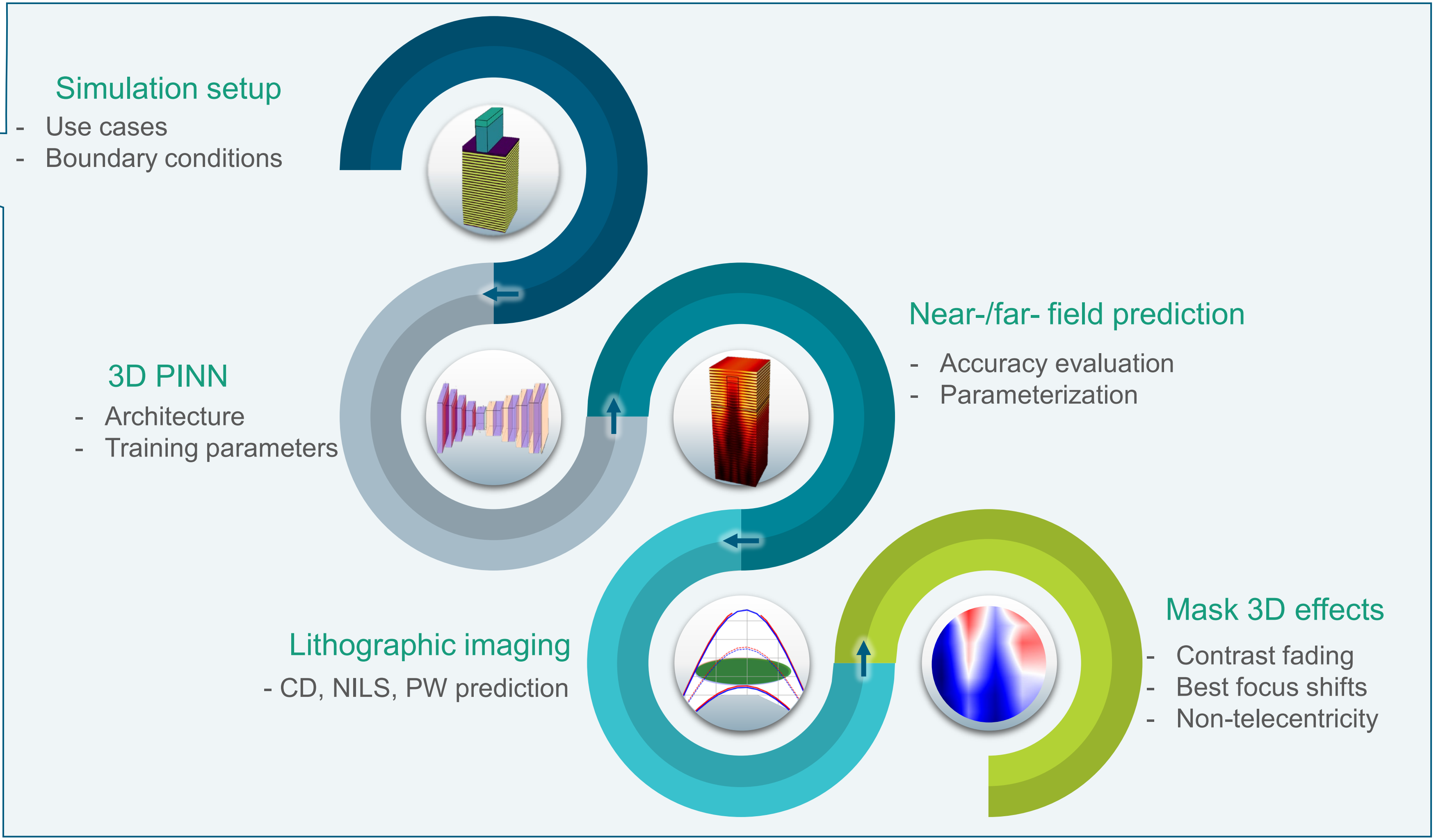
- Vlad Medvedev
- Nationality: Kazakhstan
- 2019 - 2022 **M.Sc., Advanced Optical Technologies,** Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany. Thesis title: *3D mask defect and repair based on SEM images.*
- 2022 - present **Ph.D., Computational Lithography & AI-Augmented Simulation Groups,** Fraunhofer IISB, Germany. Thesis topic: *Physics Informed Neural Networks (PINNs) for modeling of light diffraction from EUV masks and optical metasurfaces.*

Outline

Part 1: Introduction and motivation

Part 2: Workflow

Part 3: Summary and Outlook



Part 1

Introduction and motivation

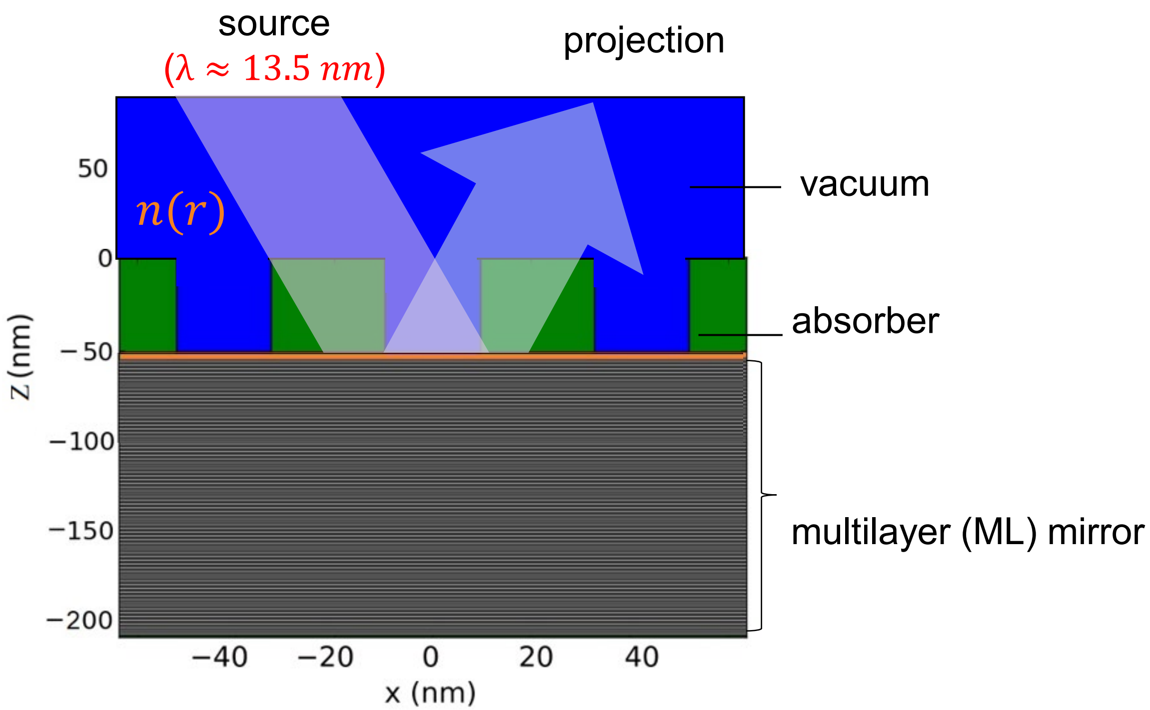
Introduction

Rigorous electromagnetic (EM) simulation in EUVL:

- Highly required for **accurate simulation of EUV imaging** and design and optimization of lithographic manufacturing processes.
- Involves solving the scattering problem through numerical approximations domain **Maxwell's equation** in the scalar form:

$$\nabla^2 E(r) + n^2(r) k_0^2 E(r) = 0$$

- Challenges:
  - modeling with the required **accuracy**.
  - modeling of **larger mask areas** with design-relevant layouts.
  - **fast** modeling.



Motivation

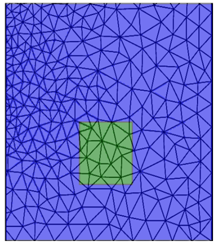
Alternative to traditional solutions

(i) Traditional numerical solvers (e.g., FEM[1], FDTD[2], RCWA[3]):

Idea: numerical techniques to iteratively solve EM simulations.

Computation time/memory amount increases for:

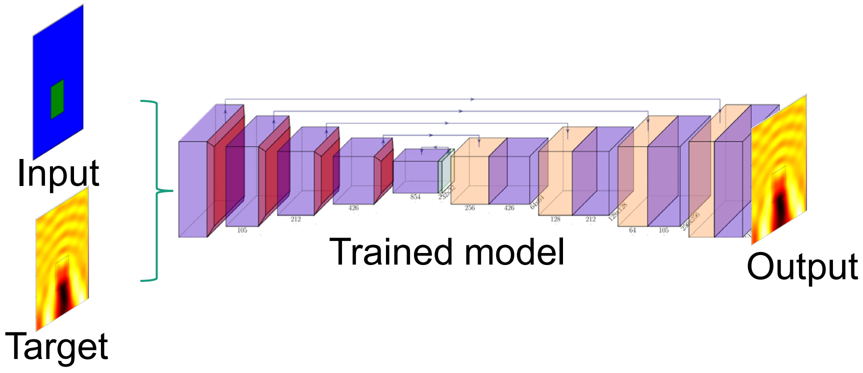
- complex physical problems.
- modeling of larger mask areas with design-relevant layouts.
- high resolution/discretization.



(ii) Data-driven deep learning (e.g., GAN[4], CNN[5]):

Idea: learns a correlation between input and output.

- Supervised based on a huge amount of expensive rigorously simulated or measured data.
- Valuable information carried by physics is ignored.



1 - Finite element method
2 - Finite-difference time-domain method
3 - Rigorous coupled-wave analysis
4 - Generative adversarial network
5 - Convolutional neural network

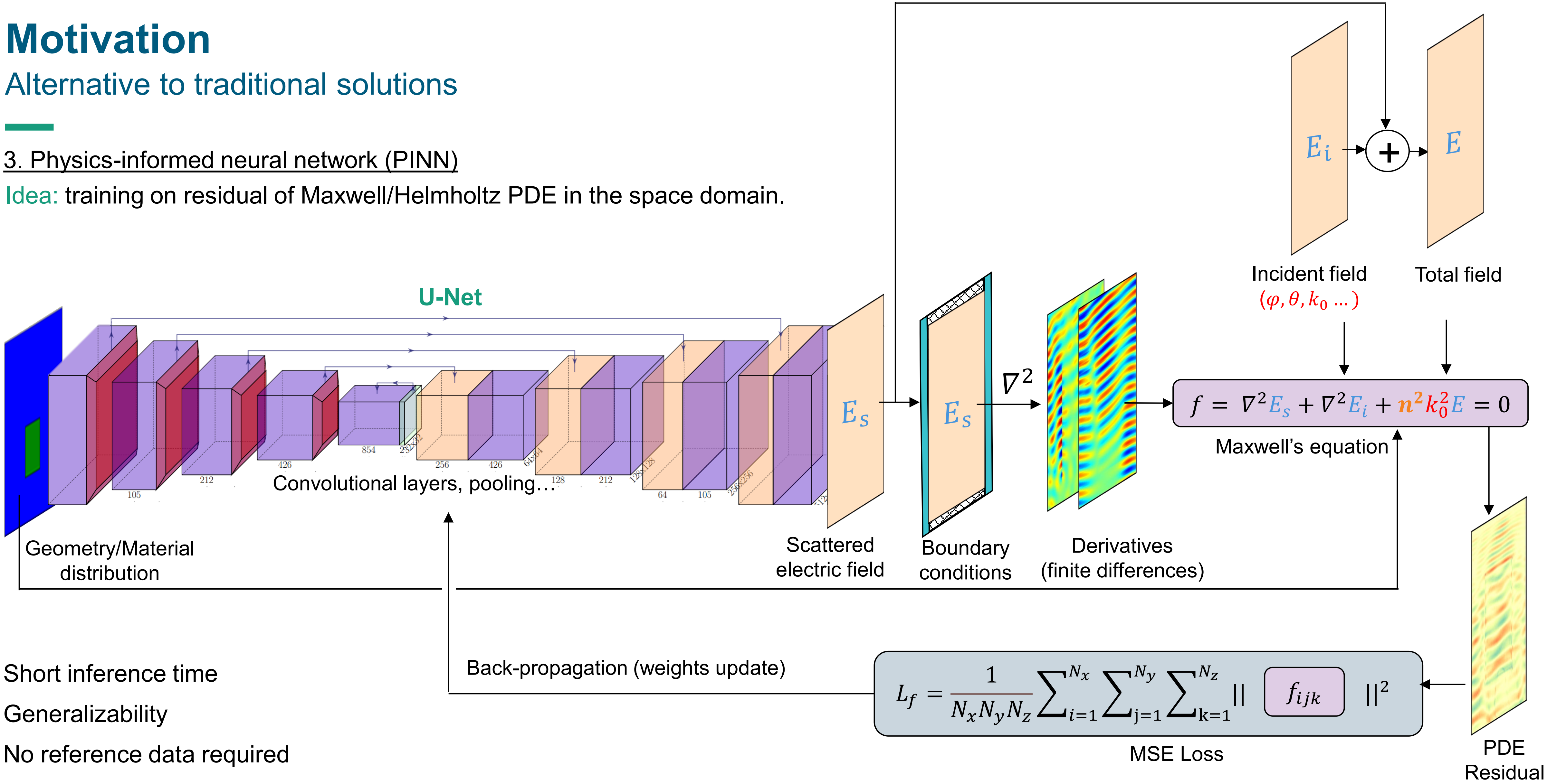
Motivation: explore the potential of (iii) physics-informed neural networks (PINN) for addressing complex optical problems in the field of EUV lithography to overcome aforementioned constraints.

Motivation

Alternative to traditional solutions

<u>3. Physics-informed neural network (PINN)</u>

Idea: training on residual of Maxwell/Helmholtz PDE in the space domain.



- ✓ Short inference time
- ✓ Generalizability
- ✓ No reference data required

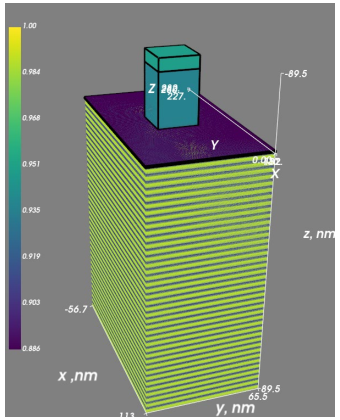
Part 2

Workflow

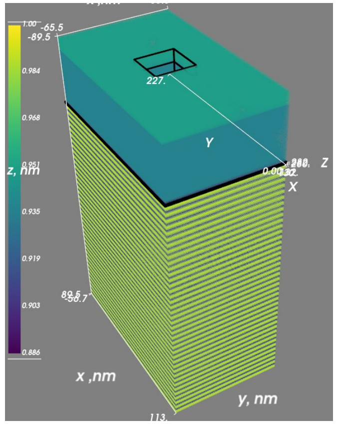
Simulation setup

Use cases

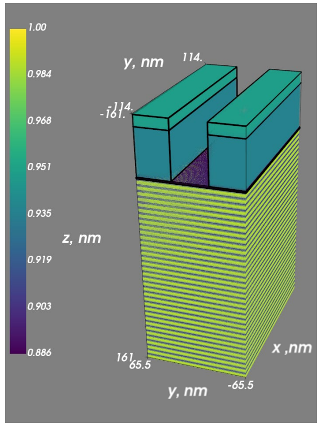
Different feature types



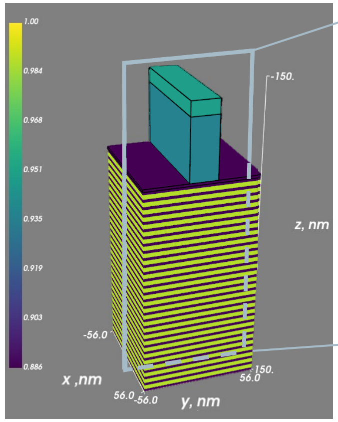
Pillar



Contact hole



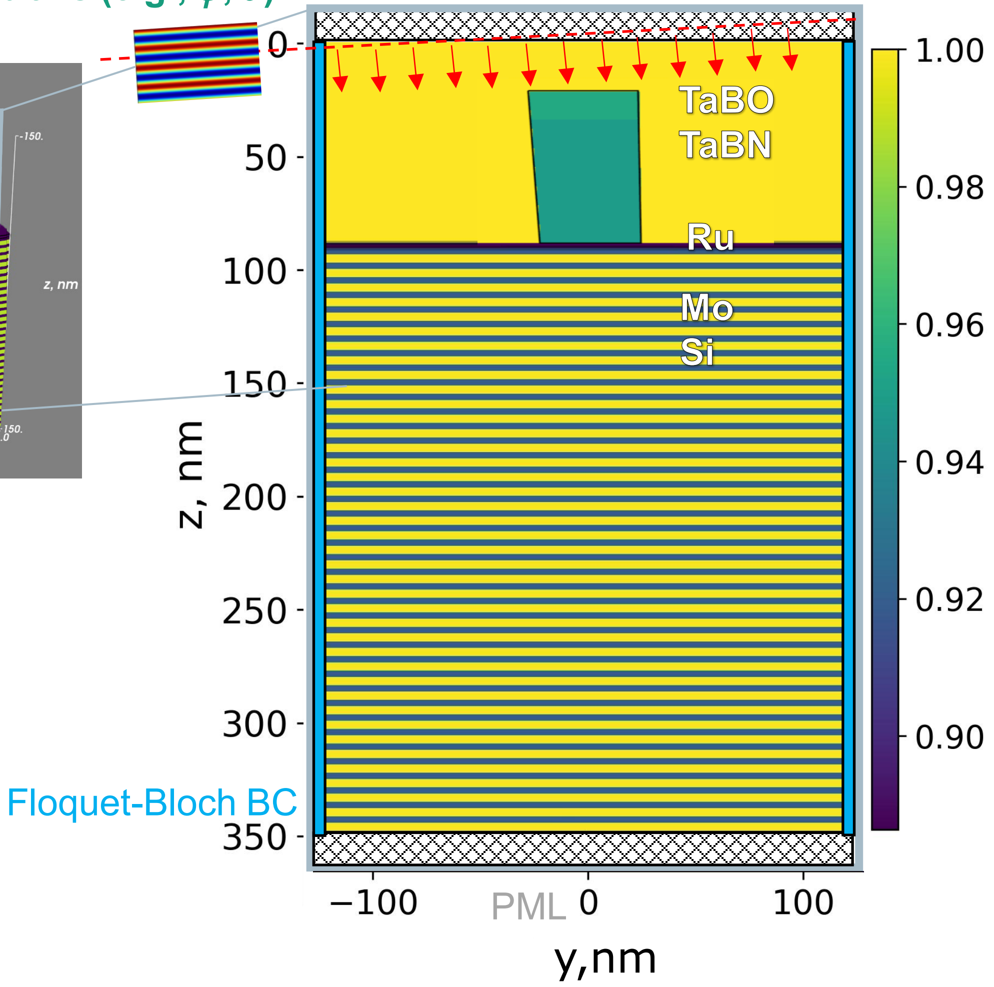
Space



Line

Different illumination directions (e.g., φ, θ)

Different mask geometries (e.g., SWA)

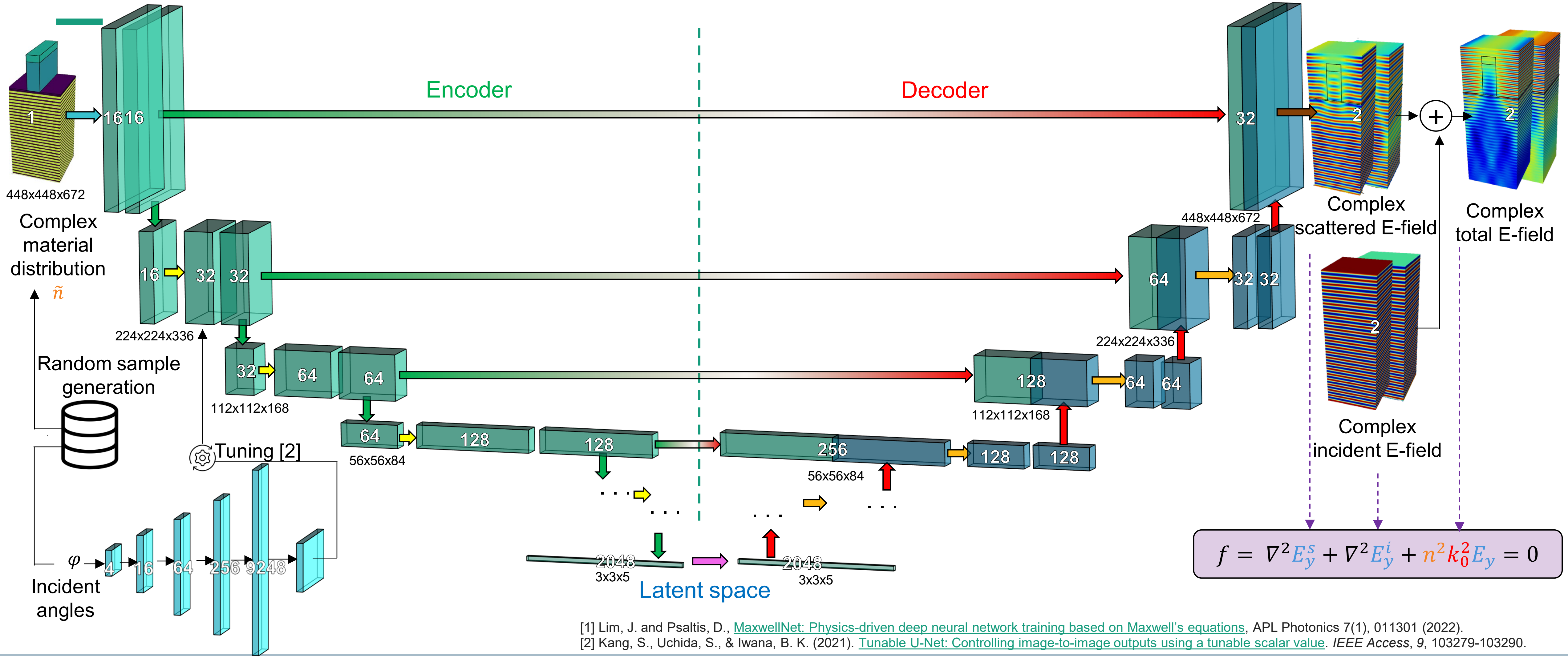


Different material properties

- Absorber: TaBN, low-n low-k, low-n medium-k, etc.
- Multilayer: MoSi, RuSi, intermixing, etc.

3D PINN

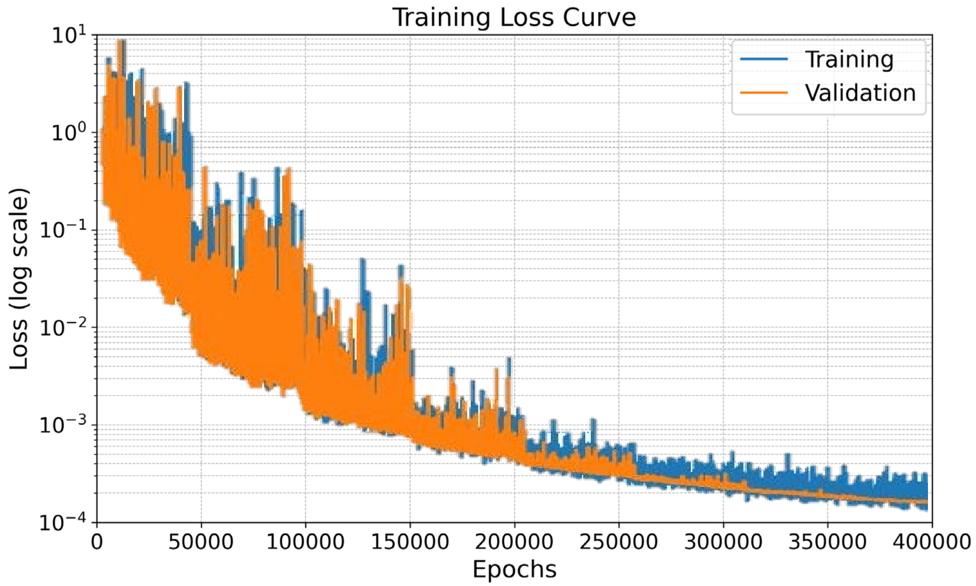
U-Net architecture [1]



[1] Lim, J. and Psaltis, D., MaxwellNet: Physics-driven deep neural network training based on Maxwell's equations, APL Photonics 7(1), 011301 (2022).
[2] Kang, S., Uchida, S., & Iwana, B. K. (2021). Tunable U-Net: Controlling image-to-image outputs using a tunable scalar value. *IEEE Access*, *9*, 103279-103290.

3D PINN

Training parameters



- Good **convergence** behavior.
- **Speedup** with respect to Waveguide solver: up to ×10000.

Table 1: Parameterization ranges.

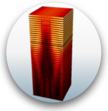
	2D
Absorber thickness, nm	[52, 80]
Feature size (wafer), nm	[20, 30]
Incident angle, °	[0, 15]
Azimuthal angle, °	[-25, 25]

Table 2: Time evaluation.

	2D	3D
Training time	~1-2 days	~7-8 days
Inference time	~1.10 ms	~100 ms

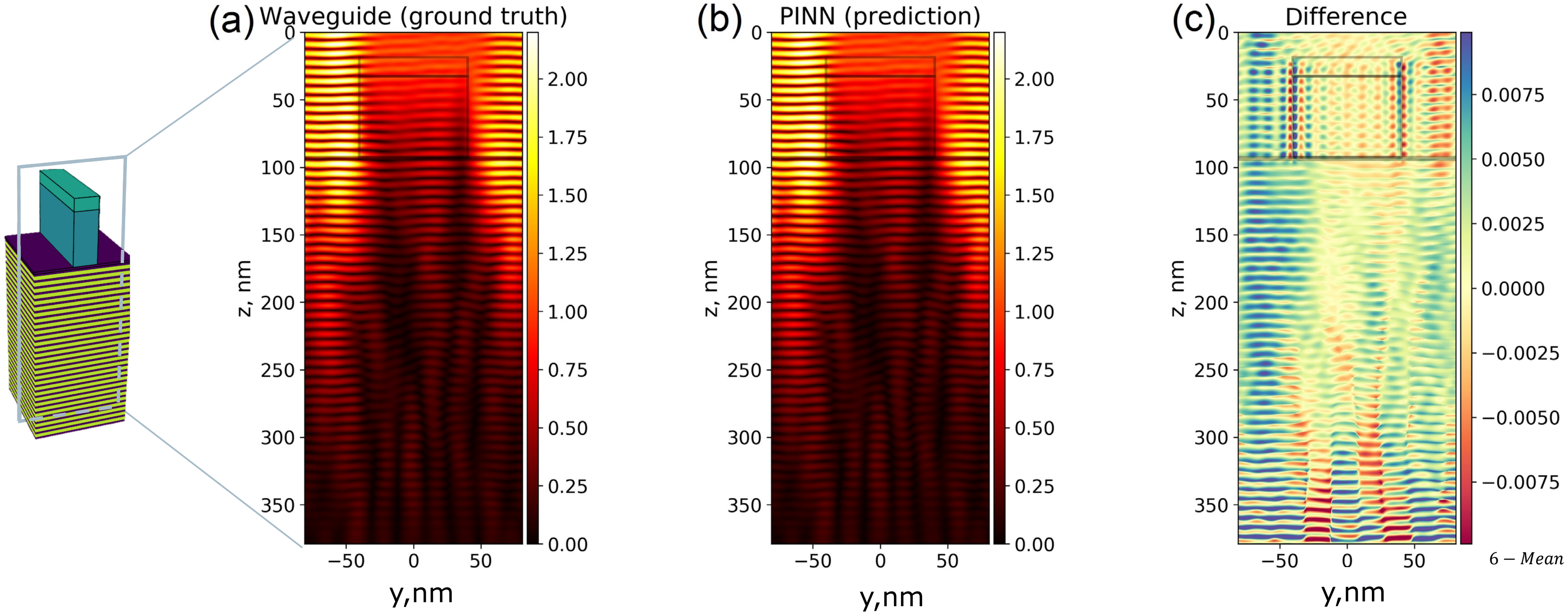
Near-field prediction

Accuracy evaluation



Input parameters:
- $\varphi = \mathbf{6°}$
- Feature type: line (hor)
- Feature size: 20 nm
- Pitch: 40 nm
- Multilayer (ML): 40xMoSi

- In contrast to other machine learning approaches, PINN is able to accurately predict the **near field** and **learn physics**.
- PINN accurately captures the physics and optical effects such as mask **shadowing** effects, **partial penetration** of EUV light into the reflective ML, and **phase deformation** by the EUV absorber.



PINN accuracy:

$$MAPE^{6}_{z=0} = 0.18\%$$

$$MAPE = 0.91\%$$

$$RMSE^{7} = 4.1E-3\text{a.u}$$

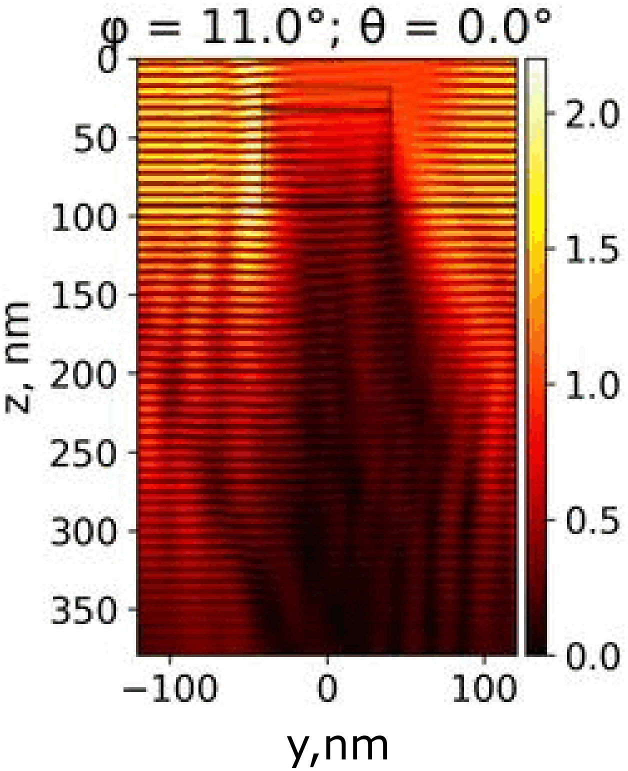
6 – *Mean absolute percentage error:* $MAPE = \frac{100\%}{N}\sum_{i=1}^{N}\left|\frac{E_{ref}-E_{pred}}{E_{ref}}\right|$

7 – *Root mean squared error:* $RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(E_{ref}-E_{pred})^2}$

Near-field prediction

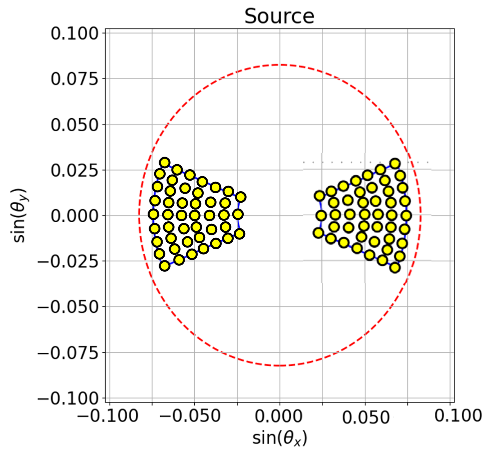
Parameterization

- U-Net architecture makes PINN well-positioned for large-scale and high-dimensional problems due to **parameter sharing via filter-based convolution operations.**
- Differently from numerical solvers, once trained, generalized PINN can simulate light scattering in **a few tens of milliseconds without re-training** and **independently of problem complexity**.



PINN model parameterized towards illumination:

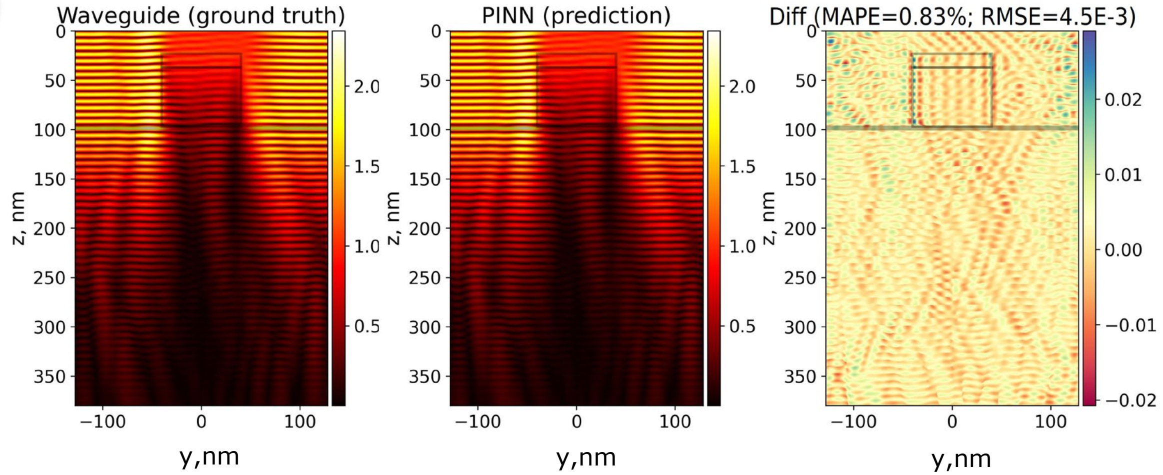
- The Hopkins approach cannot be used for correct EUV imaging simulation.
- The advantage of a trained PINN is that the imaging simulation time is almost **independent** from the number of used noHopkins points.



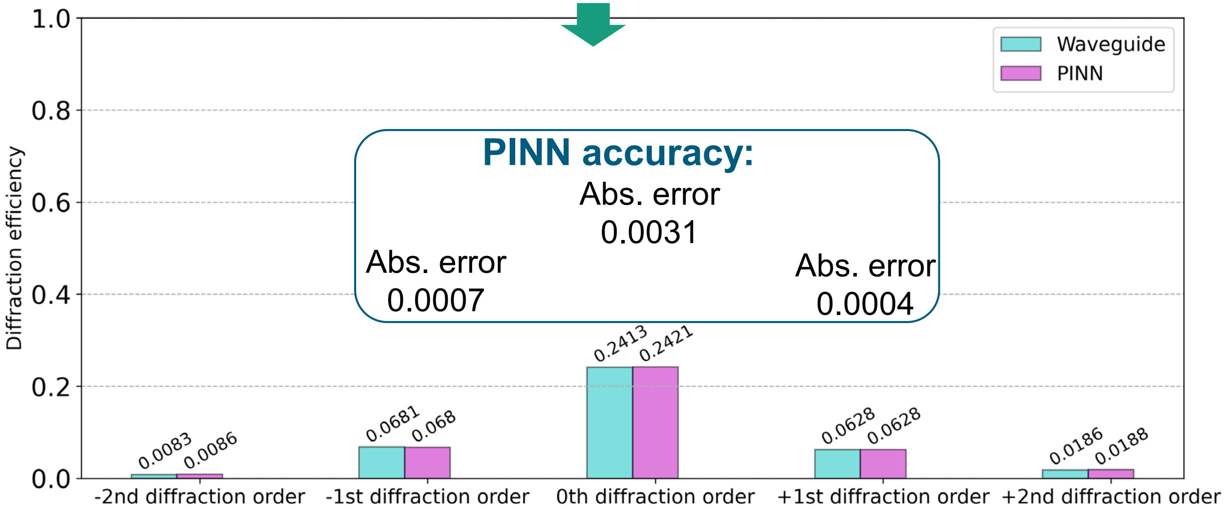
Far-field prediction

Accuracy evaluation

Input parameters:
- $\varphi = \mathbf{6}°$
- Feature type: horizontal line
- Feature size: 20 nm
- Pitch: 64 nm
- Multilayer: 40xMoSi



Near-to-far-field transformation (FT)



PINN accuracy:

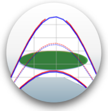
Abs. error 0.0031

Abs. error 0.0007

Abs. error 0.0004

Lithographic imaging

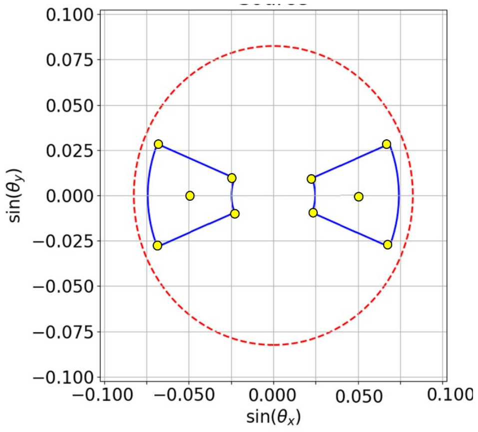
Relevant metrics

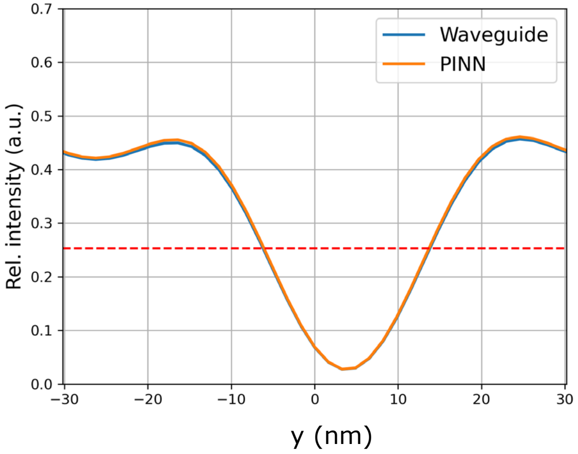


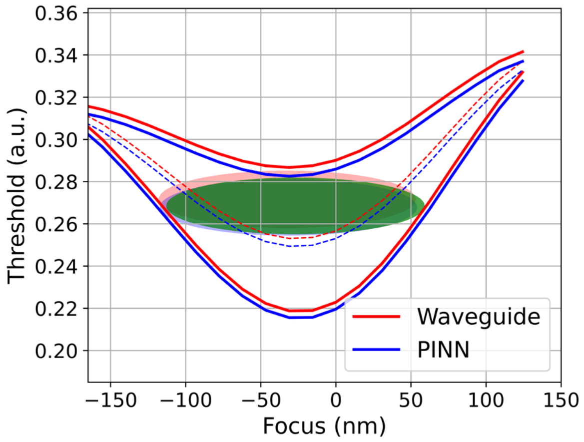
Pitch = 64 nm
Projection:
- NA = 0.33

Illumination:
- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Opening angle = 45°
- noHopkins point per pole = 5

- The overlapping green area **almost completely covers** the ellipses of both process windows → sufficient PINN's accuracy in predicting lithographic process windows.



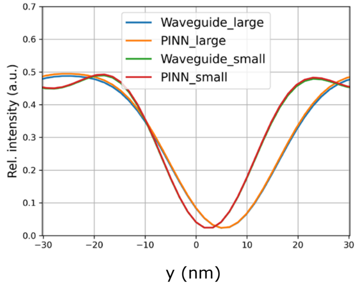




PINN accuracy:

CD_{PINN} = 19.81 nm (error 0.95%)

$NILS_{PINN}$ = 2.67 (error 0.75%)



Mask 3D effects

1. Non-telecentricity (nTC)

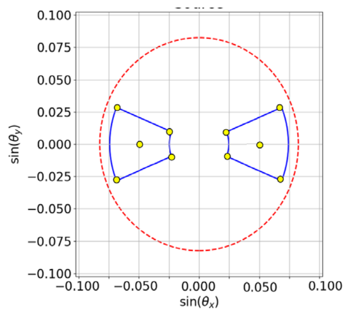
Pitch = 64 nm

Projection:

- NA = 0.33

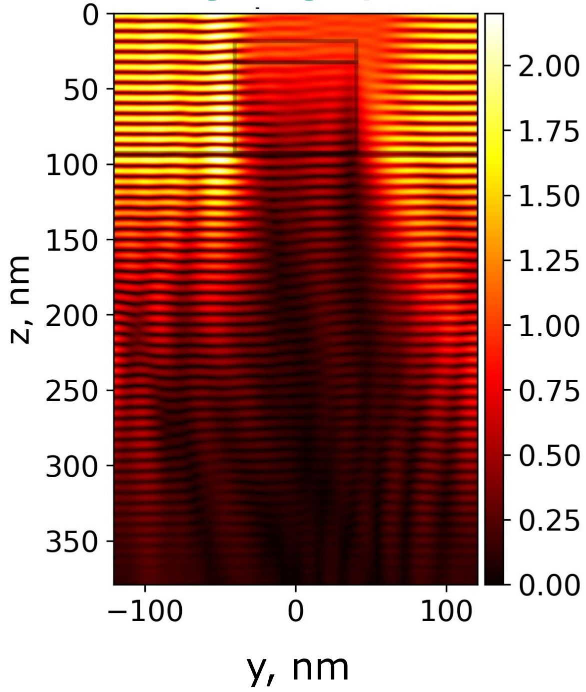
Illumination:

- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Opening angle = 45°
- noHopkins point per pole = 5

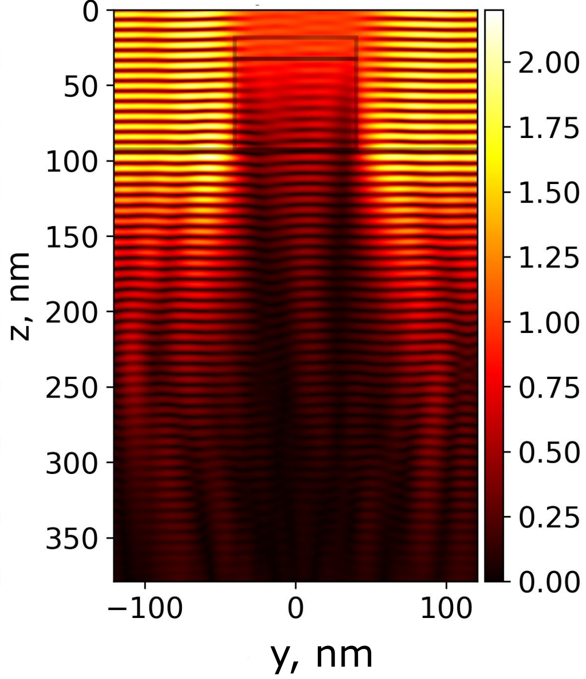


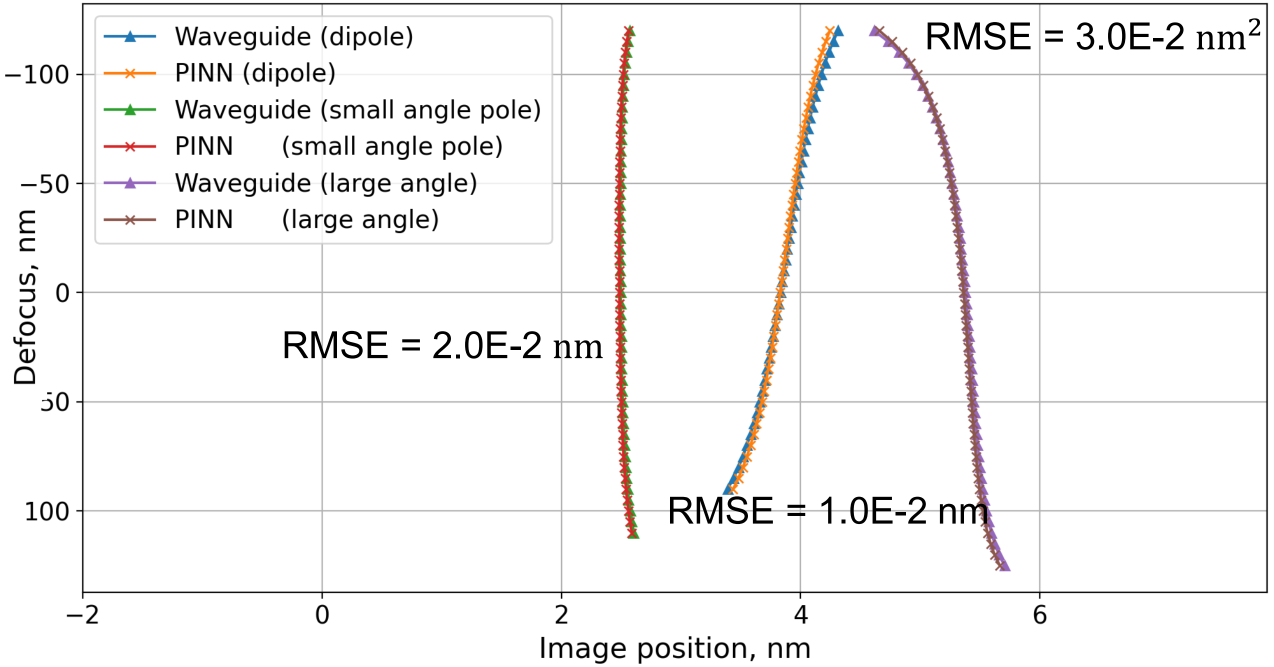
- Both 3D mask design and off-axis illumination contribute to **nTC error** → shifts of image position through focus (pattern placement errors).

Large angle pole



Small angle pole





PINN accuracy:

nTC_{PINN} = *2.77 mrad*

(error 0.72%)

Mask 3D effects

2. Contrast fading

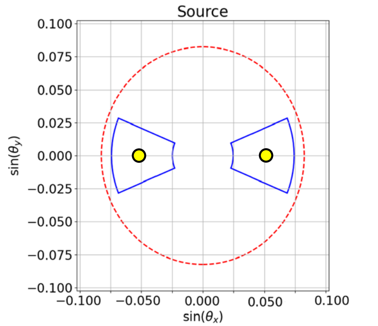
Pitch = 60 nm

Projection:

- NA = 0.33

Illumination:

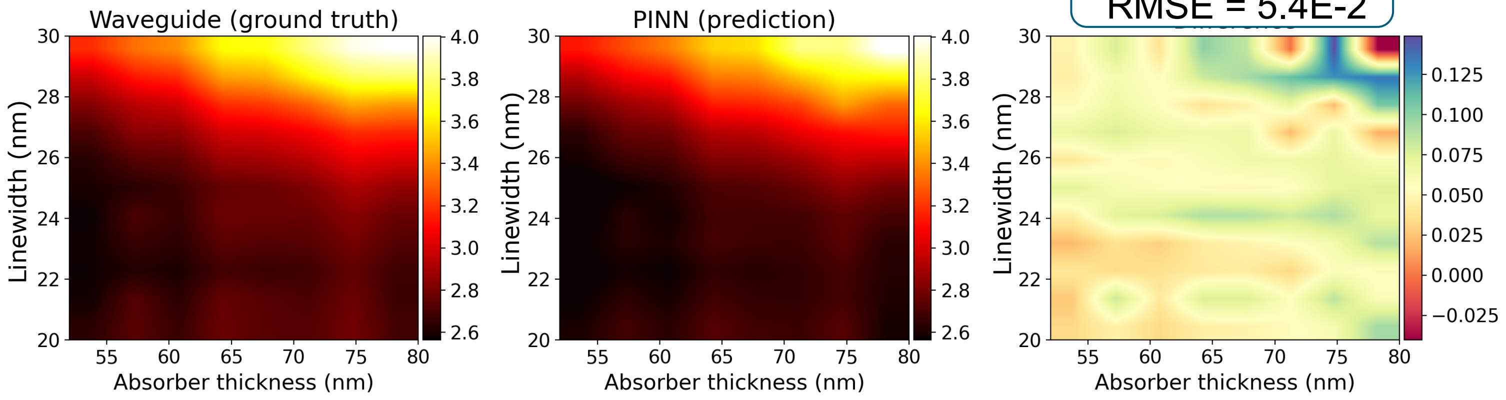
- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Opening angle = 45°
- noHopkins point per pole = 1



- Shadowing causes a shift between images from left and right poles → superposition of shifted images causes **a drop of NILS**.
- PINN explores variations of image blur vs. physical parameters in a **short time**.
- PINN can predict both diffraction order balancing and shifts of image position → **improved image** contrast through optimization.

NILS

PINN accuracy:
RMSE = 5.4E-2



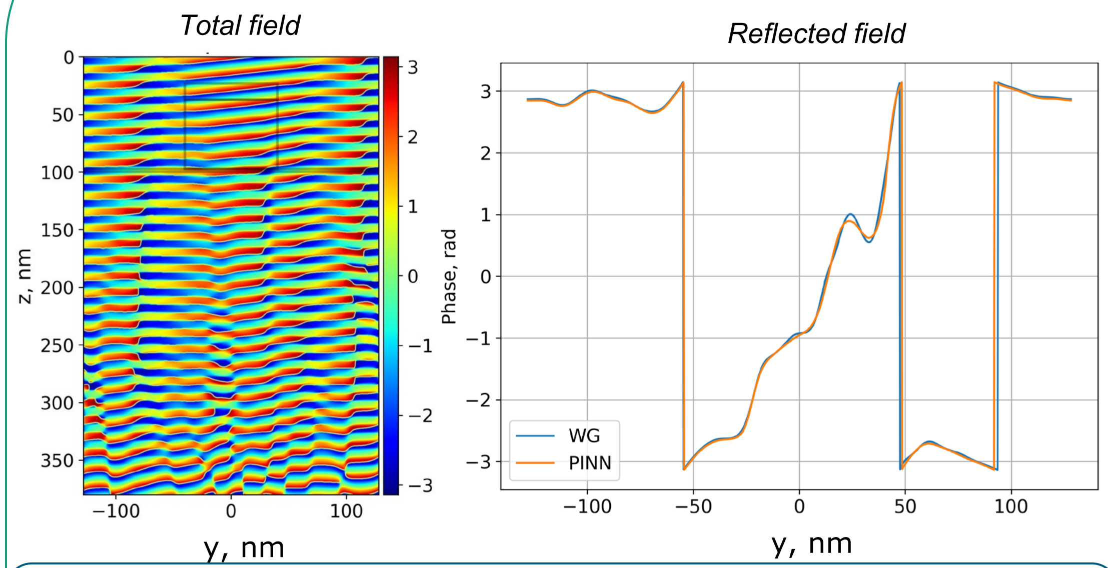
Mask 3D effects

3.1 Shift of the best focus (BF)

Input parameters:
- $\varphi = \mathbf{6°}$
- Feature type: line (hor)
- Feature size: 20 nm
- Pitch: 64 nm
- Multilayer: 40xMoSi

- Mask topography and the **phase distortion** in multilayer cause a shift of the BF position.
- PINN predicts correct phase shift between orders → therefore it can predict best focus shift versus **physical parameters** (pitch, absorber thickness, feature size).

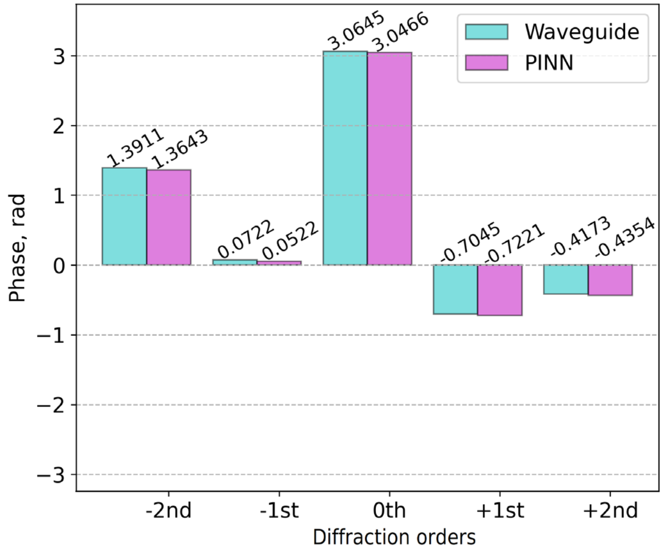
Near field: phase deformation (i)



PINN accuracy:

Phase: MSE = 1.8E-3 rad^2

Far field: asymmetric diffraction behavior (ii)



PINN accuracy:

Between -1st/0th:
$\delta(\Delta phase) = 0.07\%$

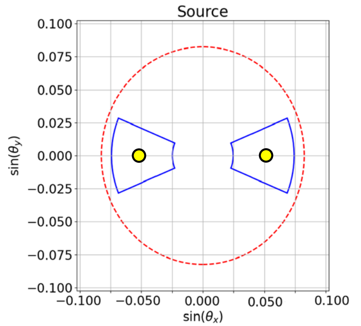
Between 0th/+1st:
$\delta(\Delta phase) = 0.01\%$

Mask 3D effects

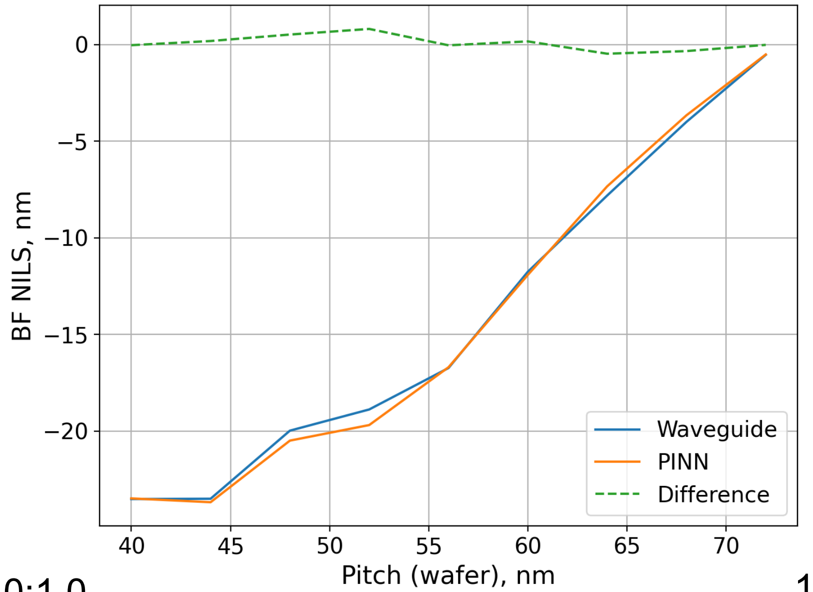
3.2 Shift of the best focus

Pitch = 60 nm
Projection:
- NA = 0.33

Illumination:
- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Opening angle = 45°
- noHopkins point per pole = 1



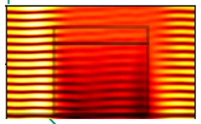
BF vs. Pitch



1.0:1.0

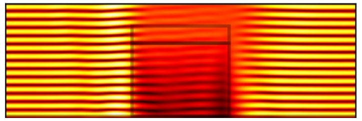
1.0:3.6

Duty ratio



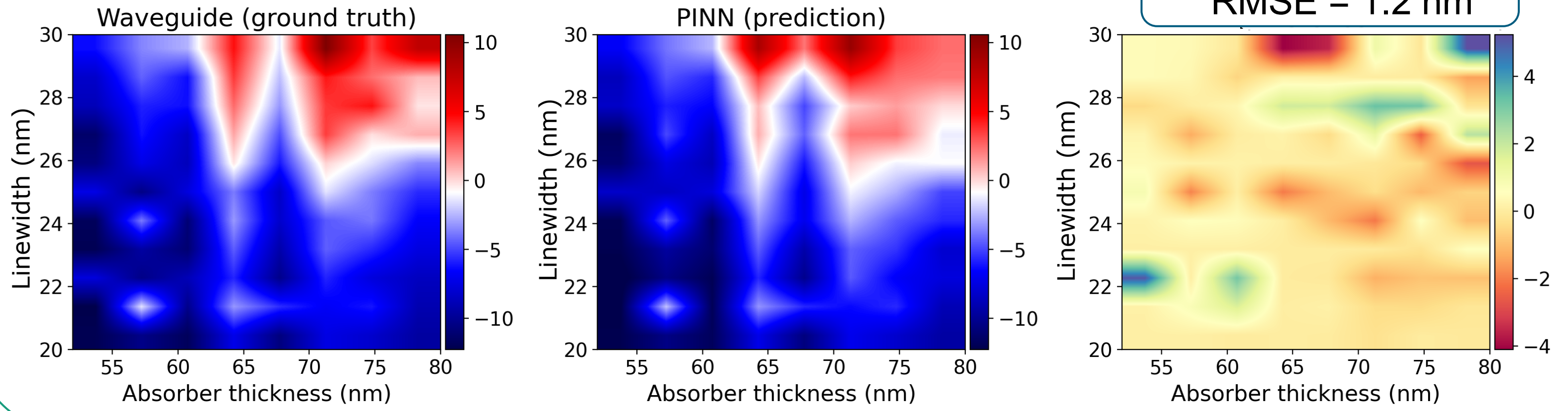
PINN accuracy:

RMSE = 9.0E-3 nm



BF vs. Size/Absorber thickness

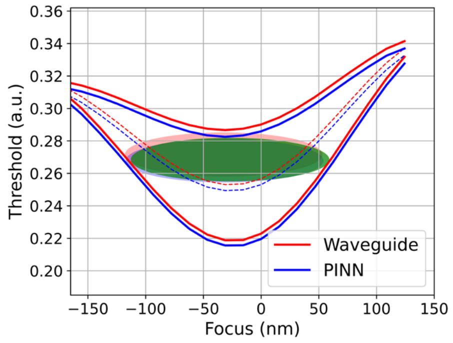
PINN accuracy:
RMSE = 1.2 nm



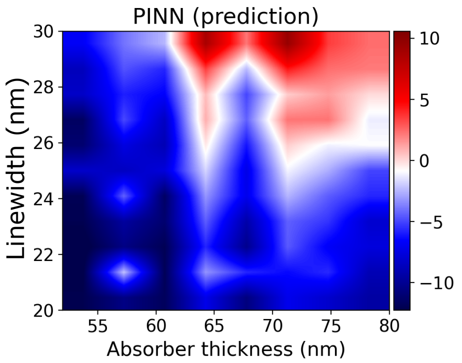
- Trained PINN can predict BF versus absorber thickness, illumination and other settings in **short time**.
- PINN captures physical effects, such as the **swing behaviour** of BF versus absorber thickness variations.

Summary

- For the first time the potential of PINN to simulate EUV light diffraction from typical reflective EUV masks was explored:
  - Good **convergence behaviour, high accuracy, and** stability.
  - Ability to **interpolate** and **generalize** across variations of EUV lithography-related parameters (illumination and mask geometries).



- PINN compared to other *machine learning* approaches:
  - is able to accurately simulate the near field.
  - learns given physics and accurately captures the optical and mask-induced 3D effects.
  - **NO experimental or rigorously simulated data** is required for training.



- PINN compared to rigorous *numerical solvers*:
  - Fast inference time (ms) → **significant speedup** (up to ×10000) w.r.t. to numerical solution.
  - Generalizability: light scattering simulation without re-training and independently of problem complexity.

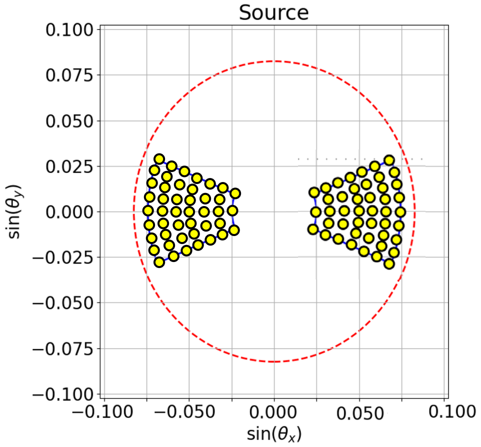
Outlook

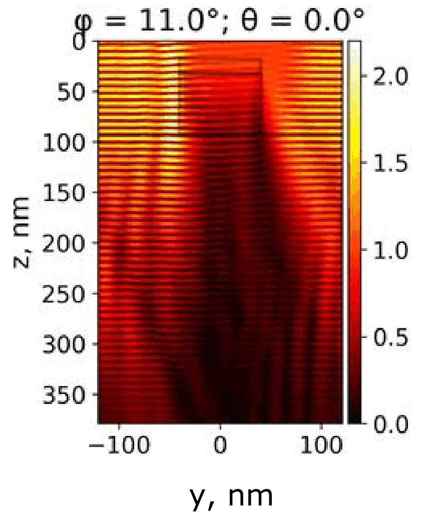
PINN for EUVL applications

- PINN-based solver, adapted for arbitrary illumination settings → imaging simulation time is almost **independent** from the number of used noHopkins points.

- Employing a vector formulation of the wave equation → investigate the ability of the PINN approach to predict the weak **polarization effects.**

- **Inverse design** → PINNs application in the OPC, SMO and ILT.





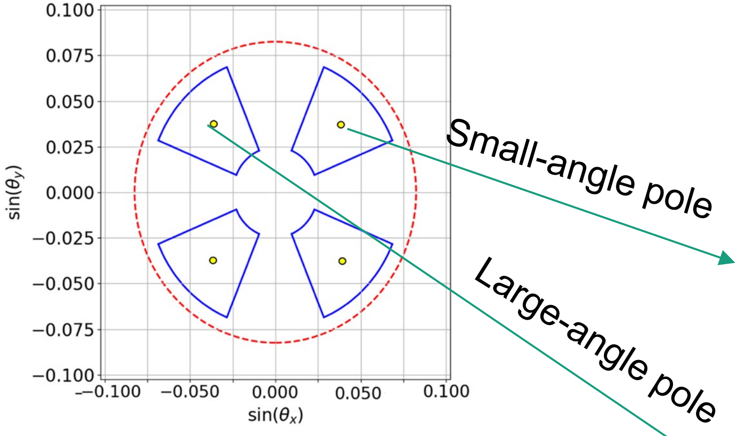
For any questions please contact: vlad.medvedev@iisb.fraunhofer.de

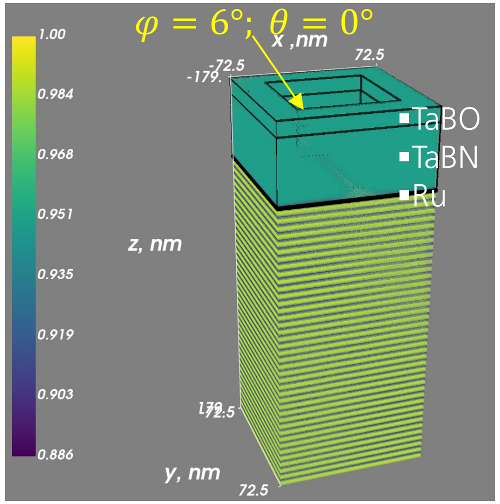
Backup

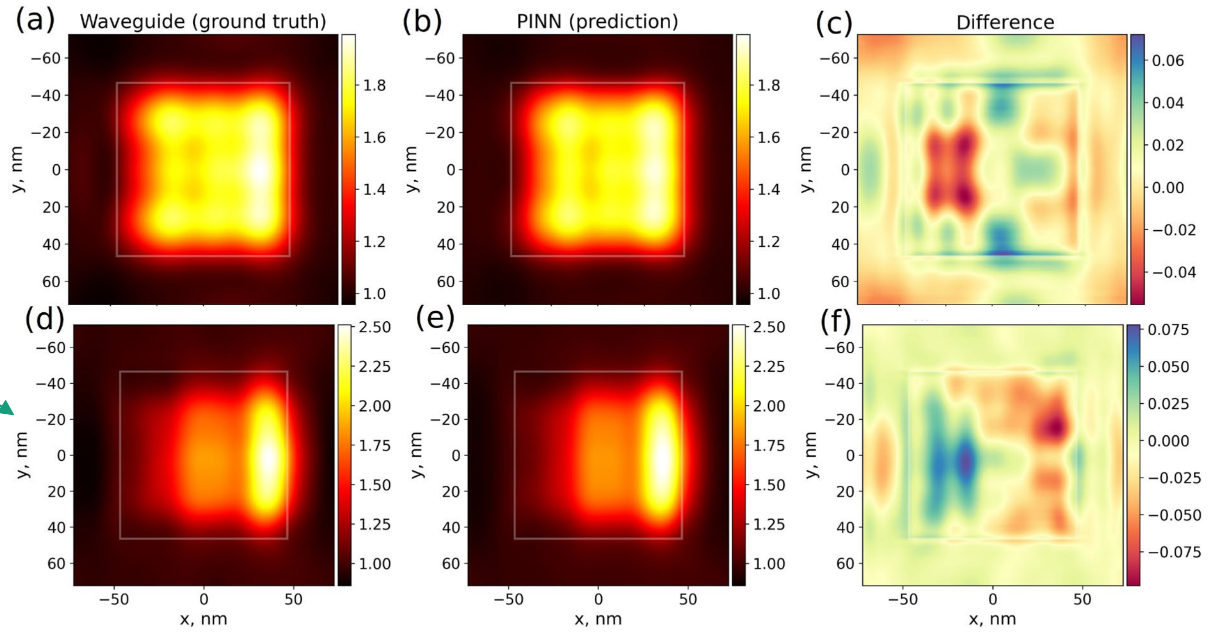
Simulation of 18 nm contact hole

Near field evaluation

Input parameters:
- $\varphi = \mathbf{6°}$
- Feature type: contact hole
- Feature size (mask): 72 nm +biasing
- Feature size (wafer): 18 nm
- Pitch: 36 nm
- Multilayer (ML): 40xMoSi







PINN accuracy:

$MAPE_{z=0} = 0.91\%$

$RMSE = 1.2E-2 \text{a.u}$

$MAPE_{z=0} = 0.95\%$

$RMSE = 1.4E-2 \text{a.u}$

Simulation of 18 nm contact hole

Lithographic imaging

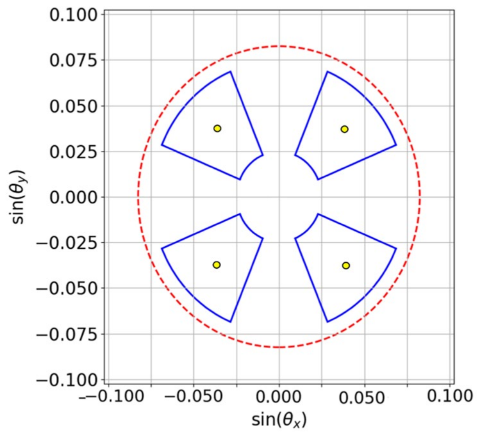
Pitch = 36 nm

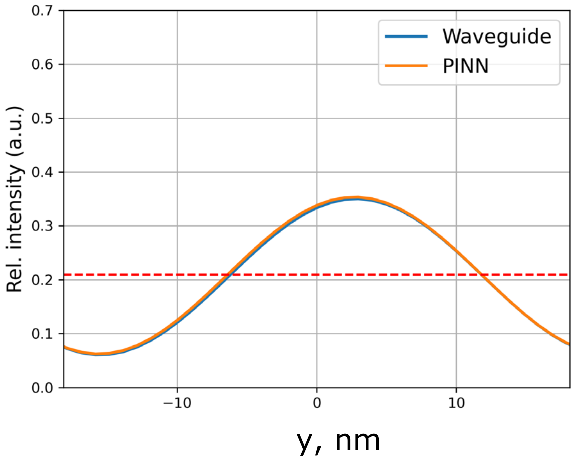
Projection:

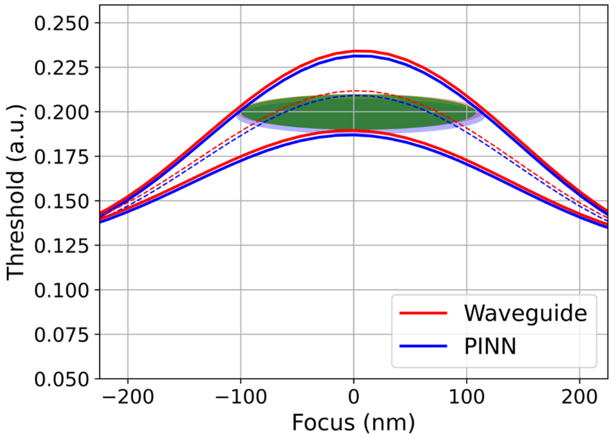
- NA = 0.33

Illumination:

- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Opening angle = 45°
- noHopkins point per pole = 1





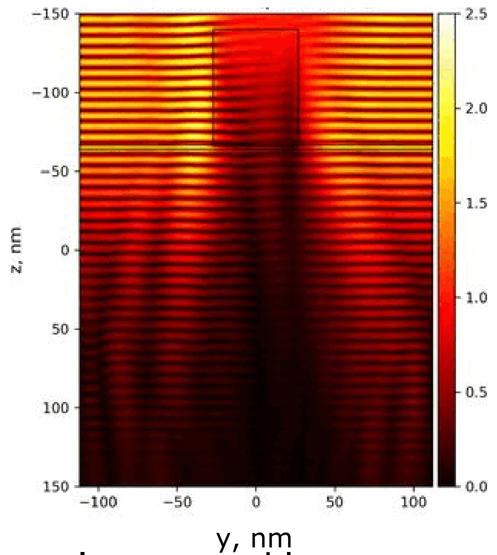


Parameter	Waveguide method	PINN	Percentage error, %
CD, nm	18.00	18.21	1.17
NILS	2.13	2.14	0.47
Best focus NILS, nm	17.39	17.90	2.93
Depth of focus NILS, nm	163.56	159.67	2.37

Near-field prediction
Parameterization

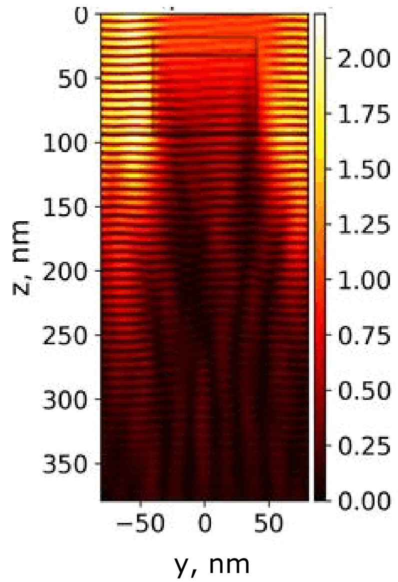
- U-Net architecture makes PINN well-positioned for large-scale and high-dimensional problems due to **parameter sharing via filter-based convolution operations.**
- Differently from numerical solvers, once trained, generalized PINN can simulate light scattering in **a few tens of milliseconds without re-training** and **independently of problem complexity**.

Absorber geometry variations



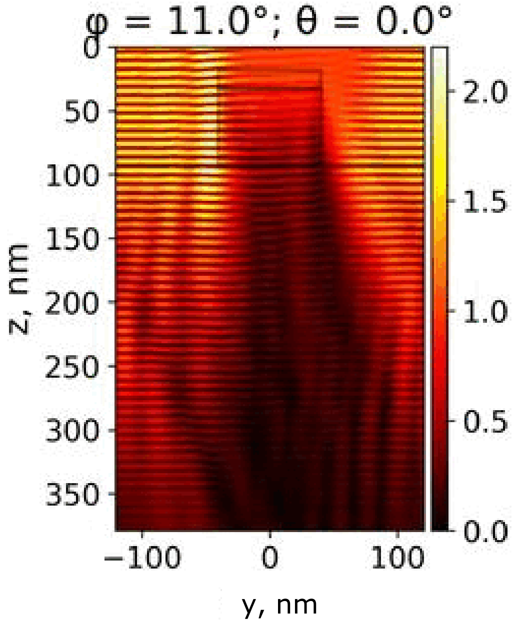
- Inverse problems.
- Topology optimization.

Pitch variations



- Studying mask 3D effects.

Illumination variations



- Partially coherent imaging simulations without the assumption of shift-invariance (noHopkins approach).
- Seamless integration with spectrum and domain decomposition methods.

3D PINN

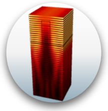
Training parameters

Table 1: Model parameters

NetworkSpecs	
Type	Convolutional Neural Network
U-Net depth	[6...8]
Filter	16
Batch size	4
Learning rate	[1E-4 … 3E-4]
Learning rate decay	Exponential; ×0.5 every 50000 epochs
Activation function	CELU
Optimization	Adam
GPU machine	2 x NVIDIA A100 80 Gb

Far-field prediction

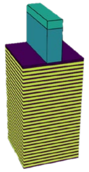
Accuracy evaluation

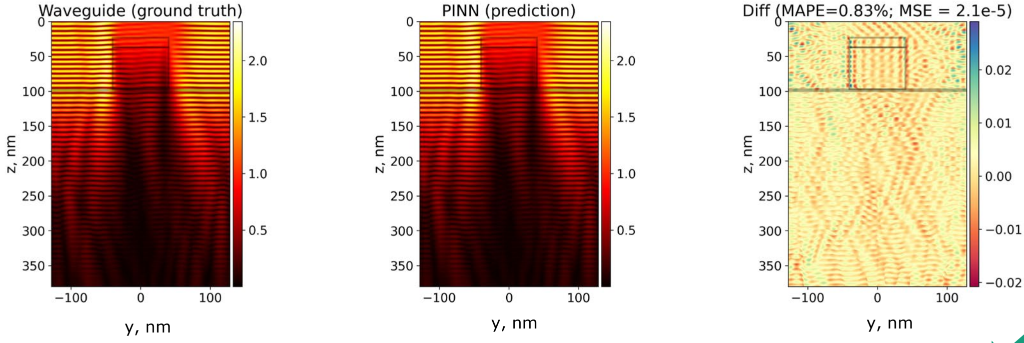


Input parameters:

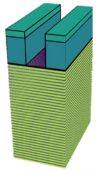
- $\varphi = 6°$
- Feature type: line/space (hor)
- Feature size: 20 nm
- Pitch: 64 nm
- Multilayer: 40xMoSi

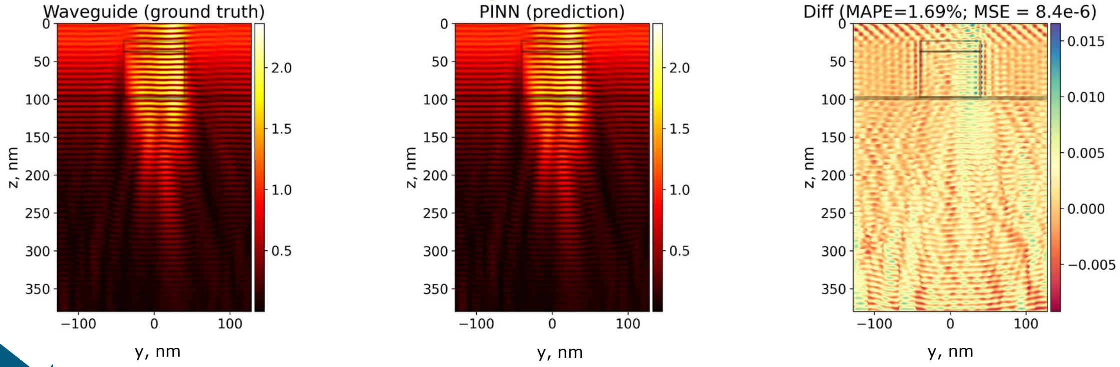
Line



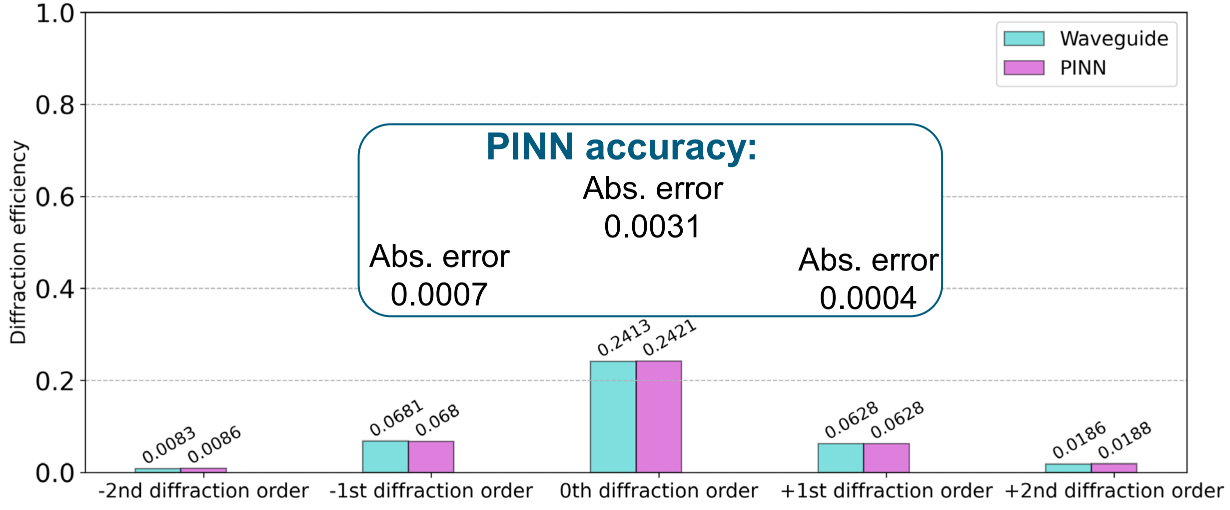


Space





Near-to-far-field transformation (FT)

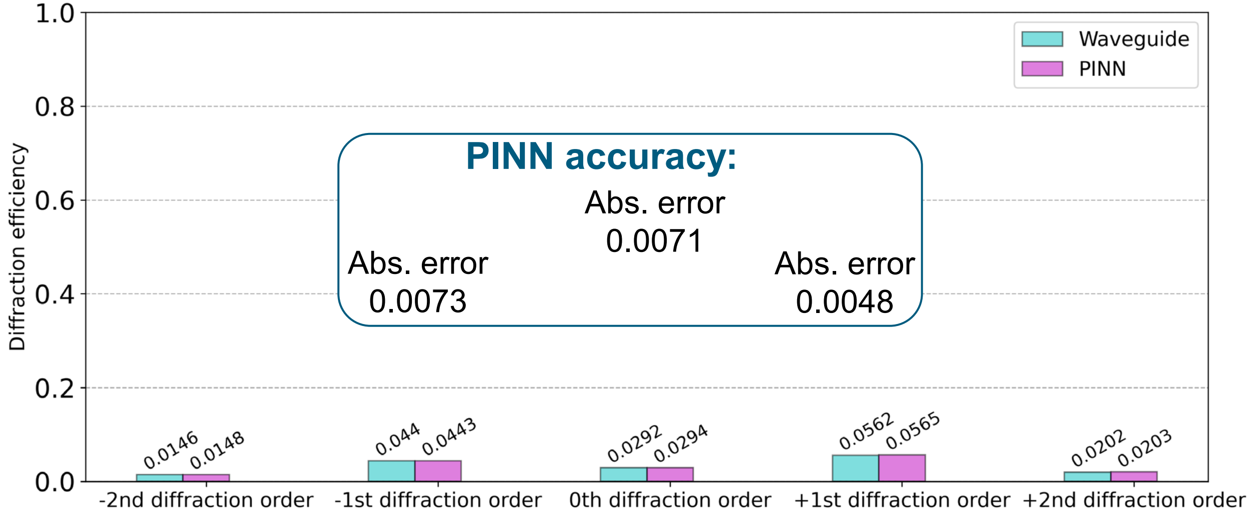


PINN accuracy:

Abs. error 0.0031

Abs. error 0.0007

Abs. error 0.0004

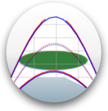


PINN accuracy:

Abs. error 0.0071

Abs. error 0.0073

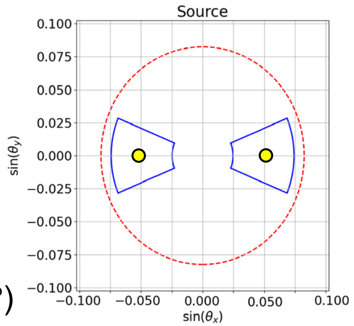
Abs. error 0.0048

Lithographic performance 

Relevant metrics

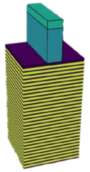
Projection:
- NA = 0.33

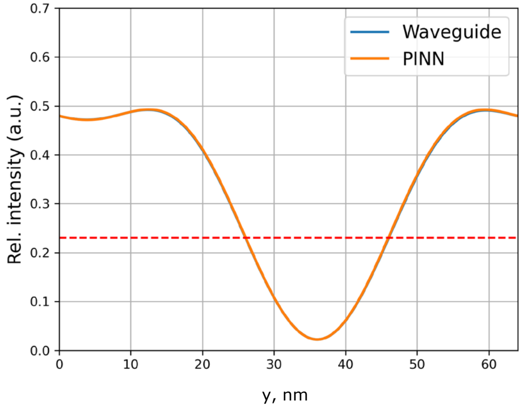
Illumination:
- Inner pole radius σ_{in} = 0.30
- Outer radius σ_{out} = 0.90
- Radial source point density = 20
- Tangential source point density = 70
- noHopkins point per pole = 1 ($\varphi \pm 2.86°$)

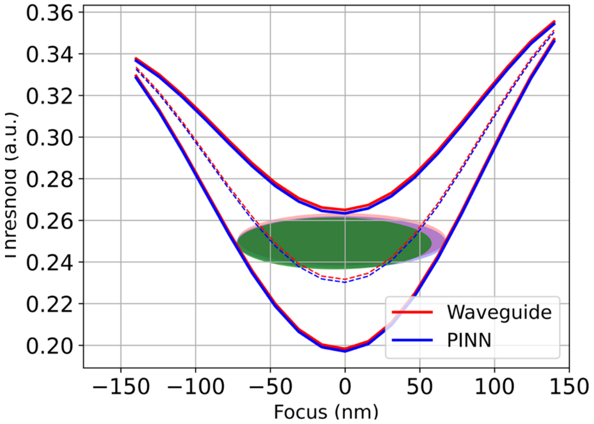


- The overlapping green area **almost completely covers** the ellipses of both process windows → sufficient PINN's accuracy in predicting lithographic process windows.

Line



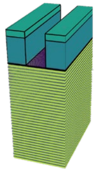


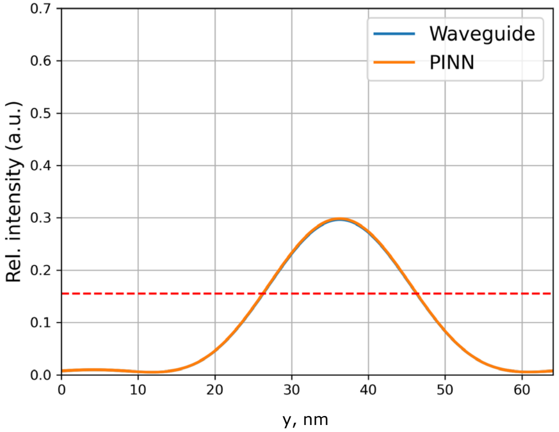


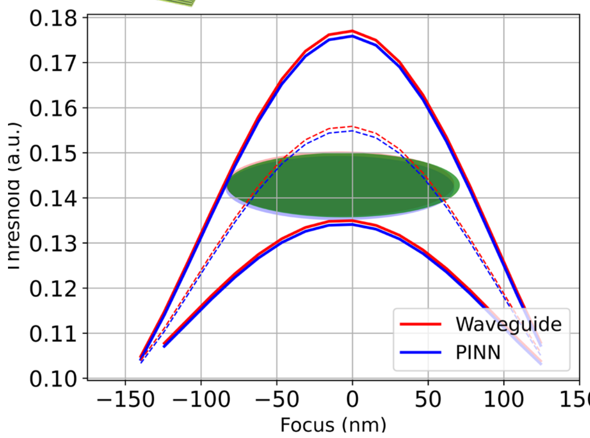
PINN accuracy:

CD_{PINN} = 19.92 nm (error 0.42%)

Space







PINN accuracy:

CD_{PINN} = 20.09 nm (error 0.47%)