Topology-Preserving Deep Learning for Structural Integrity in Optical Semiconductor Characterization at Deeply Subwavelength Resolution

Yuhan Peng[a], **Benquan Wang**[a], **Kelin Xia**[a], **Zexiang Shen**[a]

[a] *School of Physical and Mathematical Science, Nanyang Technological University, Singapore 637371, Singapore*
*Contact Authors: xiakelin@ntu.edu.sg, BENQUAN001@e.ntu.edu.sg

1. Introduction

Advancing semiconductor fabrication and development requires precise characterization of increasingly compact devices consisting of complex geometries made from diverse materials. Optical metrology and imaging are non-destructive, label-free, and real-time techniques but face the fundamental resolution restriction to half the wavelength (λ) of light.

While deep learning offers promising super-resolution capabilities, traditional neural networks employing pixel-wise prediction mechanisms fundamentally struggle with structural integrity in semiconductor characterization. These isolated pixel mispredictions, though minor in overall accuracy metrics, can falsely indicate defects or breaks in reconstructed semiconductor features, rendering quality control decisions unreliable and potentially compromising manufacturing yield. Here, we propose a topology-enhanced deep learning framework for optical semiconductor characterization that systematically incorporates topological constraints through specialized loss functions derived from persistent homology principles.

Our approach enhances attention to structural integrity in regions where pixel-wise methods alone plateau. Experimental validation demonstrates high-fidelity optical imaging of semiconductor features as small as 0.16λ with approximately 10% improved correlation compared to conventional pixel-wise methods, while dramatically reducing false structural discontinuities. This non-invasive, topologically enhanced optical characterization paradigm opens new possibilities for high-precision semiconductor quality control and smart manufacturing processes where geometric integrity at the nanoscale is paramount.

1.1 Related work

Deep learning has been widely applied to optical imaging, with recent work such as [1][2] using U-Net for nanoparticle and nanowire imaging. However, its pixel-wise loss function often leads to structural discontinuities, failing to preserve the connectivity of fine structures such as nanowires.

To address structural consistency, topological data analysis (TDA) has been incorporated into deep learning models. The work of [3] introduced a topological loss function for segmentation networks. By matching the Betti number, this topological loss-based model can preserve local topology, i.e., the predictions will always share the same topology with the ground truth. The model offers significant advantages in situations where topological information is severely degraded by noise.

In this work, we first employ TDA integrated deep learning for optical semiconductor characterization, which can address the fundamental changes when the predictions and ground truth share the same Betti numbers but differ in spatial distribution or shape. Furthermore, our model employs extended persistent homology model [4], thus it is free from the limitations of single filtration strategy, such as failing to characterize the full complexity of topological structures in diverse imaging datasets.

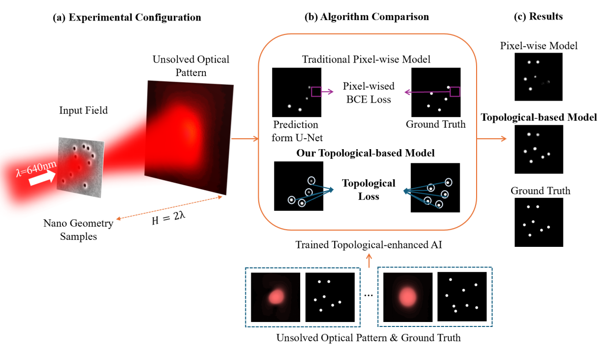

Fig. 1: Comparison of traditional pixel-wise models and our topological-based model for optical pattern reconstruction. (a) The input field, generated by nano geometry elements in a size of 0.16λ (100nm) illuminated by a plane wave with a wavelength of 640nm, produces an unresolved optical pattern at a propagation distance of $H = 2\lambda$. (b) Traditional pixel-wise models, such as U-Net with binary cross-entropy (BCE) loss, struggle to reconstruct fine structural details, leading to incomplete or fragmented predictions. Our proposed topological-based model with a topological loss function ensures structural consistency by preserving key topological features, e.g. Betti numbers. (c) The output comparison demonstrates that our method more accurately reconstructs the ground truth compared to the traditional model.

2. Methodology

We frame our task as a binary segmentation problem, where each pixel in a diffraction-limited optical input image is labeled to reconstruct deeply subwavelength features in the super-resolved output. This approve enables the recovery of structural details that exist beyond the conventional diffraction limit.

2.1 *Network Architecture*

We employ an encoder-decoder U-Net architecture, specifically a scientifically modified U-Net specialized for optical imaging, as proposed in our previous work [5]. The encoder extracts hierarchical features from the low-resolution input, while the decoder reconstructs a super-resolved binary segmentation output. Unlike conventional architectures that optimize only pixel-wise accuracy, our model incorporates a topology-aware loss function to enhance structural correctness.

2.2 *Topological Loss Function L_{topo}*

Inspired by the Euler Characteristic Transform (ECT) [6] and Persistent Homology Transform (PHT) [7], we leverage persistence diagrams from multi-directional filtrations as sufficient statistics for shape modeling due to their injectivity. Thus, our topological loss is computed as follows:

1. Directional Transform [6]: Given a simplicial complex $K \in \mathbb{R}^n$, we fix a directional unit vector $\omega \in \mathbb{R}^d$. This direction induces a simplex-wise function:
$$f_\omega : K \longrightarrow \mathbb{R}, \quad \sigma \longrightarrow \max_{v \in \sigma} \langle v, \omega \rangle$$
where $\langle x, y \rangle = \sum x_i y_i$ denotes the standard dot product of the vectors x and y. To enhance topological feature extraction, we apply filtrations along multiple directions: $\omega \in \{\binom{1}{0}, \binom{-1}{0}, \binom{0}{1}, \binom{0}{-1}\}$ which ensure a robust characterization of topological structures.
2. L_{topo}: We compute persistent homology based on cubical complex on the transformed images using the filtrations defined above and summarize their topological information through persistent diagrams. The topological loss function is defined as the Wasserstein distance between the persistence diagrams Dgm of the predicted (f) and ground truth images (g):
$$L_{topo}(f, g) = W(Dgm(f), Dgm(g))$$
which measures structural discrepancies in a Lipschitz-continuous manner [8]. This formulation ensures that our loss function is both differentiable and robust to small perturbations.

2.3 *Training and Optimization*

We train our model using a composite loss function that combines a standard pixel-wise loss with our proposed topological loss:
$$L_{loss} = L_{bce} + \lambda L_{topo}$$
where L_{bce} is standard BCE loss and λ is a balancing parameter. We use a stochastic gradient descent optimizer with adaptive learning rates to ensure stable convergence.

3. **Results**

We evaluated the performance of our U-Net model using two loss functions: (1) BCE loss and (2) our proposed topological loss function. The prediction results are displayed in Figure 2, where we compare the pixel-wise and our topology-based models' segmentation outcomes. Our proposed method demonstrates superior structural fidelity compared to the pixel-wise model, achieving enhanced preservation of topological features, reduced noise, and better positional alignment.

Model	MSE ↓	Pearson Correlation ↑
Pixel-wise	0.017	0.61
Our Model	**0.0145**	**0.72**

Table 1: Comparison of model performance.

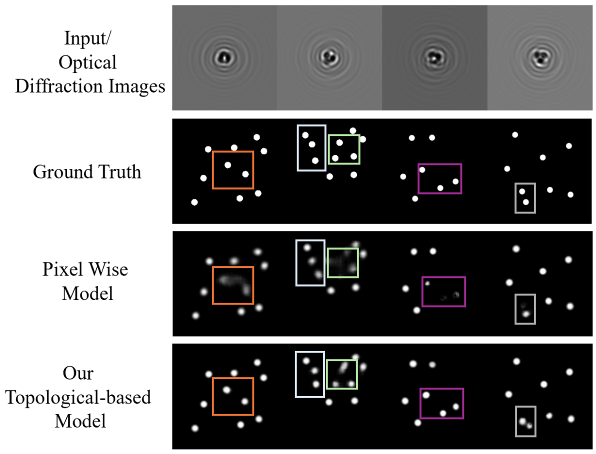

Fig. 2: Comparison of segmentation results between a pixel-wise model and our topology-based model. The first row presents the input optical diffraction images. The second and third rows show the predictions from both models respectively, and the fourth row displays the corresponding ground truth. Our topology-based model produces more accurate and structured segmentation than the pixel-wise approach, as highlighted.

Quantitative comparison of the models is provided in Table 1. Our model achieves a Mean Squared Error (MSE) of **0.0145** and a Pearson correlation coefficient of **0.72**, outperforming the pixel-wise model, which has an MSE of 0.018 and a Pearson correlation of 0.61. These results further highlight the effectiveness of our topology-based approach in improving segmentation accuracy and preserving relevant structural features.

4. **Conclusion**

Our results demonstrate that incorporating topological constraints into deep learning models significantly improves structural fidelity in super-resolution imaging. By leveraging multi-directional filtrations and persistence-based loss functions, our approach provides a robust solution for preserving both geometric and topological integrity in complex optical datasets.

Acknowledgments

This work was supported by the Singapore National Research Foundation (Grant No. NRF-CRP23-2019- 0006), the Singapore Ministry of Education (Grant No. MOE2016-T3-1-006)

References

[1] Tianjie Yang, Yaoru Luo, Wei Ji, and Ge Yang. Advancing biological super-resolution microscopy through deep learning: a brief review. *Biophysics Reports*, 7(4):253–266, 2021.

[2] Xin Hu, Xixi Jia, Kai Zhang, Tsz Wing Lo, Yulong Fan, Danjun Liu, Jing Wen, Hongwei Yong, Mohsen Rahmani, Lei Zhang, and Dangyuan Lei. Deep-learning-augmented microscopy for super-resolution imaging of nanoparticles. *Optics Express*, 32(1):879–890, Jan 2024.

[3] Xiaoling Hu, Fuxin Li, Dimitris Samaras, and Chao Chen. Topology-preserving deep image segmentation. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.

[4] David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Extending persistence using poincaré and lefschetz duality. *Foundations of Computational Mathematics*, 9(1):79–103, Feb 2009.

[5] Benquan Wang, Ruyi An, Eng Aik Chan, Giorgio Adamo, Jin-Kyu So, Yewen Li, Zexiang Shen, Bo An, and Nikolay I. Zheludev. Retrieving positions of closely packed subwavelength nanoparticles from their diffraction patterns. *Applied Physics Letters*, 124(15):151105, 04 2024.

[6] Elizabeth Munch. An invitation to the euler characteristic transform. *The American Mathematical Monthly*, 132(1):15–25, Jan 2025.

[7] Robert Ghrist, Rachel Levanger, and Huy Mai. Persistent homology and euler integral transforms. *Journal of Applied and Computational Topology*, 2:55 – 60, 2018.

[8] Peter Skraba and Katharine Turner. Wasserstein stability for persistence diagrams. *arXiv*, 2020.