Evolution-based EUV Scatterometry fuelled by Machine Learning Diffraction Predictions for 3D Nanoscale Semiconductor Structures

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Extreme ultraviolet (EUV) scatterometry is a promising candidate for in-line dimensional metrology of advanced nanoscale 3D semiconductor devices. A key challenge for deploying EUV scatterometry in practice is the solution of the inverse problem: reconstructing device geometries from measured diffraction signatures. Although machine-learning methods have shown strong potential for scatterometric reconstruction, most published approaches have focused on relatively simple structures described by only a few parameters. In contrast, realistic 3D device architectures are represented by many more parameters, making robust reconstruction substantially more challenging.

In this work, we present a reconstruction framework that combines a neural-network surrogate model with differential evolution for geometry retrieval. The surrogate is trained to emulate finite element method (FEM) simulations and rapidly predict diffraction intensities from geometric parameters, thereby greatly reducing the computational cost of repeated forward evaluations. Differential evolution then uses this fast forward model to efficiently explore the high-dimensional geometric parameter space and identify geometries that best reproduce the measured signature

Compared with both direct inverse neural networks and earlier hybrid approaches based on surrogate forward models with fitting algorithms, the proposed method provides greater robustness for complex experimental reconstructions. Direct inverse models often misinterpret measurement data because real experimental data differ from training simulations due to process-induced variations, simplified geometric representations, and measurement noise. In contrast, hybrid methods based on other fitting schemes such as Levenberg–Marquardt are more susceptible to becoming trapped in local minima in high-dimensional parameter spaces. By combining a neural-network surrogate with differential evolution, our approach addresses both challenges, enabling robust and efficient reconstruction of complex geometries from experimental data.

We demonstrate the method performance on an EUV photomask sample whose geometry is described by 11 parameters. To the best of our knowledge, this exceeds the geometric complexity previously reported for successful reconstruction using either conventional optimization-based approaches or machine-learning-based methods. This result highlights the ability of the proposed framework to handle significantly more realistic and challenging structures than those considered in earlier studies.

By coupling the speed and accuracy of neural-network surrogates with the global search capability of evolutionary optimization, the proposed framework provides a scalable and robust route to accurate reconstruction of complex 3D device geometries, supporting EUV scatterometry as a viable in-line metrology technique for current and future semiconductor technologies.