Supporting Information

Manuscript Title

Deep Learning Based Prediction of Fabrication-Process-Induced Structural Variations in Nanophotonic Devices

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Information

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Number of Figures: 2
Number of Tables: 0

Generating the Training Structures

The dataset of structures used to train and test the CNN predictor model was created by generating random 2D patterns with various Fourier transform based filters, as shown by the two examples in Fig. S1. This is a quick way of generating features like those of a topologically optimized photonic device. A randomized matrix is first generated to create the base distribution of pixels between core (silicon) and cladding (silica). A Fourier transform and low-frequency centering is then applied to the initial random distribution. For seven of the generated patterns, a low-pass filter (as shown in Fig. S1b) is applied to remove the high-frequency structural components (small features) and keep the low-frequency components (large features). For each of the seven patterns, a differently sized filter is applied to generate differently sized features. The other eight patterns were generated with band-pass filters (as shown in Fig. S1f) to create more-uniform features and increase the variability in the training data. The filtered Fourier components are transformed back into the spatial domain before a final, binarization stage is applied. To expand the dataset, two instances of each pattern were generated, creating 30 images in total.

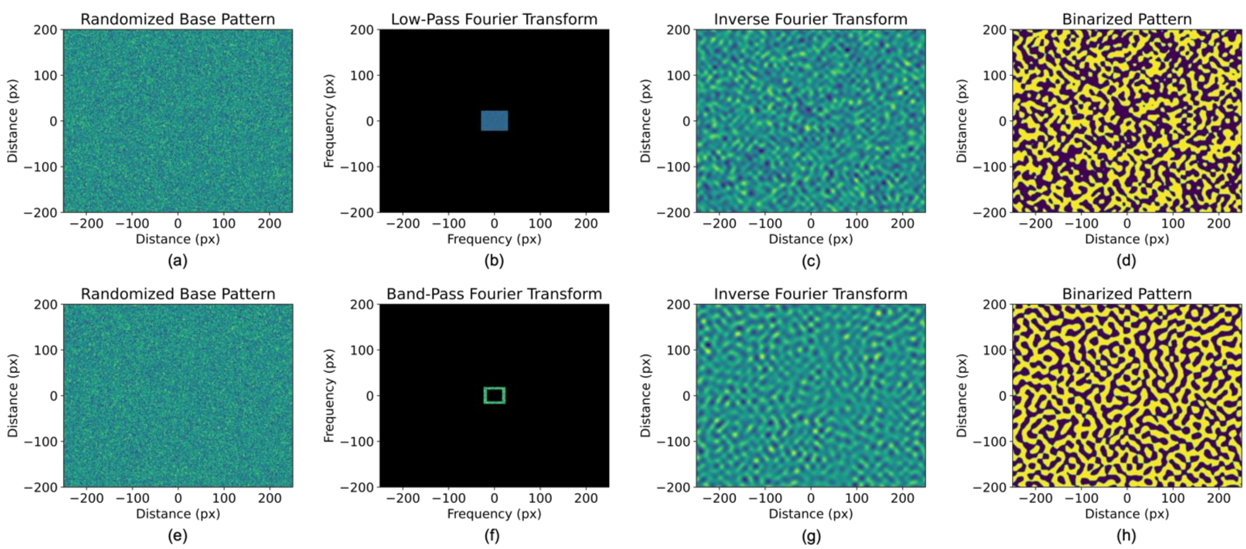

Figure S1 – Example process steps of the pattern generation process. The (a) initial, randomized base pattern, its (b) Fourier transform with a low-pass filter applied, the (c) subsequent inverse Fourier transform, and (d) the final, binarized pattern. (e–h) Corresponding figures for an example that uses a band-pass filter instead.

Image Preprocessing

The GDS and SEM images are preprocessed to prepare the dataset for training, as outlined in Fig. S2. For each structure, the GDS image is preprocessed by adjusting the scale of values from 0 (silica) to 1 (silicon) and cropping its boundaries to the outside edges of the structure. The corresponding SEM image is cropped in the same way before being resized to match the preprocessed GDS image. Both the SEM and GDS images are then padded by 100 pixels to space the boundary features away from the edges. Without this step the model cannot determine if the boundary features are cut off or if they continue past the image edges.

The SEM images require further preprocessing to match the binarization of the GDS slices. In the SEM, the edges of the structures tend to "glow" more than the rest of the structure due to charging of the nonconductive sample during the electron beam imaging step; this causes difficulties for the thresholding/binarization process. We clamp high pixel values to a value closer to the center of the silicon structures to create a more uniform color profile. Then, because different areas of the same pattern can have slightly different color profiles (again, due to charging effects of the SEM imaging), we cannot use a simple threshold value to distinguish between silicon and silica. Instead, we use an adaptive method, called Otsu's thresholding,[1] which finds suitable thresholds throughout the image. A Gaussian blur, with a filter size of 5 x 5 pixel^2 is applied before thresholding to reduce noise that can otherwise carry over.

The GDS and SEM images are then cut into 128 x 128 pixel^2 slices, in overlapping steps of 32 pixels, to fill out the dataset. For the 30 images taken, this process creates 50,680 examples for the model training/testing. The size of the slice and the step size can be modified to potentially achieve better training accuracy. The images can also be rotated and/or mirrored to artificially create more data and potentially improve the performance of the model.

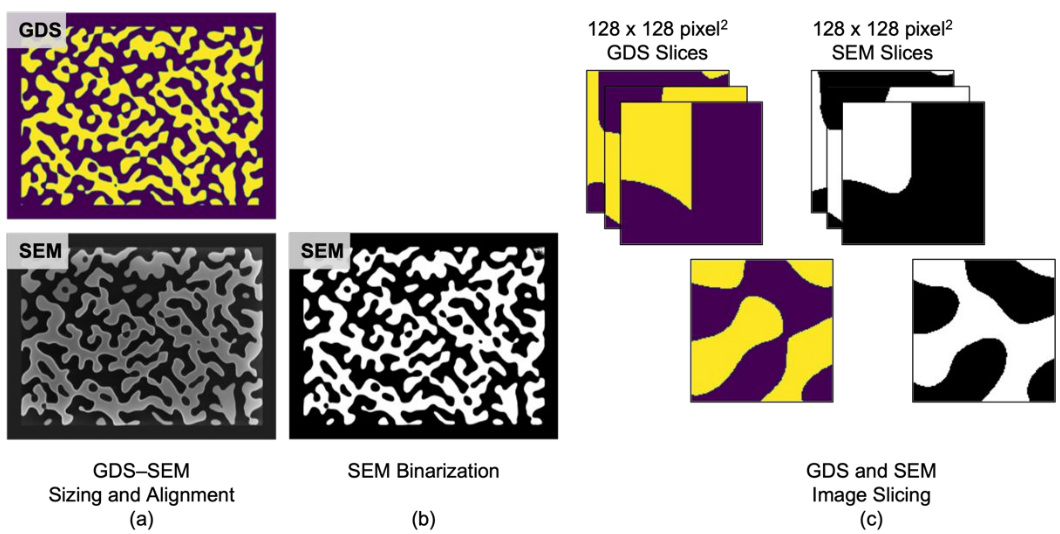

Figure S2 – GDS and SEM image preprocessing for training/testing the CNN model. (a) The GDS and corresponding SEM are cropped, scaled, and aligned to each other. (b) The SEM is binarized. (c) The GDS and SEM are cut up into overlapping 128 x 128 pixel^2 slices.

References

[1] Otsu, N. A threshold selection method from gray-level histograms. *IEEE Trans. Syst., Man, Cybern. Syst.* **1979**, *9* (1), 62–66.