Adaptive Design of EUV Scatterometry through Efficient Bayesian Inference

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ABSTRACT

Extreme ultraviolet (EUV) scatterometry offers non-destructive, chemically specific, and high-resolution metrology for nanoscale structures in modern technology. Typically, EUV scatterometry experiments are conducted with fixed arbitrary designs or fixed optimal designs. Here, we re-formulate EUV scatterometry as a closed-loop Bayesian adaptive experiment where measurement design and inference are performed sequentially using a Sequential Monte-Carlo (SMC) sampler. We first demonstrate efficient and accurate Bayesian inference using SMC sampler. Then we extend this methodology to design sequential measurements with Bayesian Adaptive Experiment Design (BAED), where we aim to extract the maximum amount of information with the fewest measurements. In a simulated experiment probing a $1\ nm$ Hf grating buried under $70\ nm$ of amorphous silicon, adaptive experiment design yielded sensitivity as low as $0.1\ nm$ and $0.1\ g/cm^3$ after 50 total measurements.

Keywords: extreme ultraviolet (EUV), EUV scatterometry, EUV diffractometry, Bayesian inference, Sequential Monte-Carlo (SMC), Bayesian Adaptive Experiment Design (BAED)

1. INTRODUCTION

Modern fabrication methods enable the creation of nanostructured and precisely engineered features, from ultrathin transistor oxides to nanoscale interconnects, that enable advanced electronic devices. Yet fabrication remains a highly time- and resource-intensive sequence of hundreds of tightly constrained steps, and the vanishingly small tolerances of modern devices place new demands on metrology to identify process deviations or faults at the earliest possible stage.

Extreme ultraviolet (EUV, $\lambda \approx 10$–100 nm) scatterometry is an emerging metrology modality attracting growing attention for its ability to measure geometric parameters such as critical dimension (CD), line width roughness (LWR), line edge roughness (LER) and compositional properties with depth resolution extending to several hundred nanometers. [1,2] EUV scatterometry can serve as a valuable complementary metrology technique to more common approaches such as atomic force microscopy (AFM), scanning electron microscopy (SEM), ellipsometry, and scanning transmission electron microscopy (STEM), with significant advantages of being nondestructive and requiring no special sample preparation.

In an EUV scatterometry measurement, EUV light is focused to a small spot ($\sim 2\ \mu m$) and reflected from a sample. In the case where the sample corresponds to periodic structures the reflected light corresponds to a discrete first-and-higher order diffraction spots, which are recorded on a CCD or CMOS detector. By varying the angle of incidence or the illumination wavelength, the resulting diffraction efficiencies form a characteristic curve that can be modeled using methods such as rigorous coupled wave analysis (RCWA)[3]. When this model is fit with an appropriate optimization routine, the technique provides accurate unit-cell-averaged measurements of the structures within the illuminated region. However, extracting this information with high fidelity requires careful control of the illumination conditions and precise knowledge of the optical properties of the materials involved.

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Recent work from our team has shown that the Fisher information matrix can be used to identify the experimental conditions that maximize information about a specific sample, opening new pathways for applying statistical methods in EUV metrology [4]. In Section 2, by using a sequential Monte-Carlo sampler (SMC[5]), we explore implementation of methods in Bayesian statistics to two separate aspects of experimental EUV scatterometry: parameter estimation and adaptive experiment design. Section 2.1 showcases the efficiency and accuracy of parameter estimation with Bayesian inference and an SMC sampler. Section 2.2 extends our capability to adaptive design of EUV scatterometry experiments and demonstrates potential for high sensitivity to parameters of a 1D buried Hf grating. In Section 3, we discuss our results, outlining the feasibility of this new formulation of EUV scatterometry and establishing its validity. These methods and results are important because they enable a fast feedback loop for inference and design that can be applied to important samples with large numbers of parameters to increase measurement sensitivity.

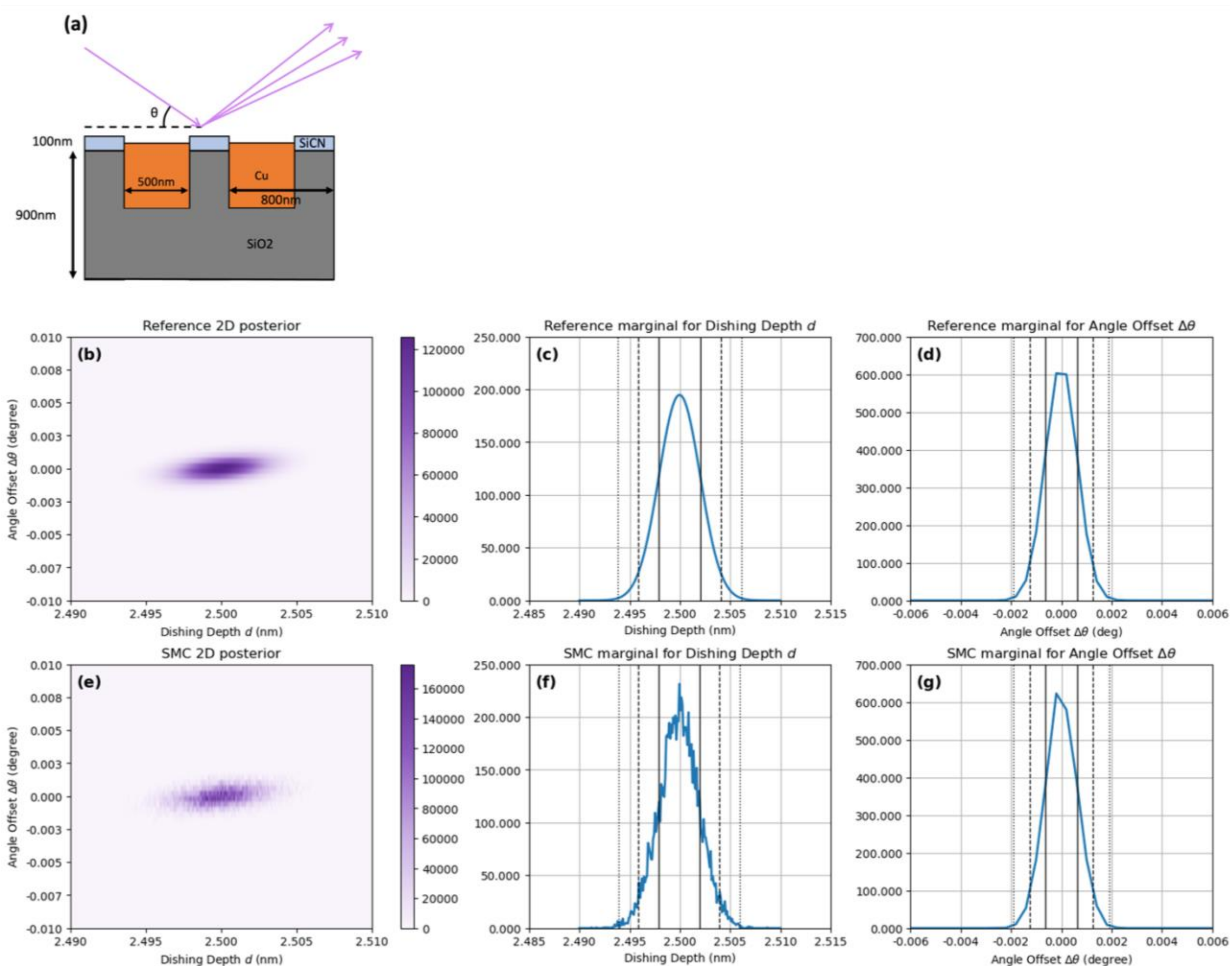

Figure 1, Comparison of reference localized Monte-Carlo Bayesian inference and sequential Monte-Carlo Bayesian inference. (a) Simulated copper interconnect schematic. Angle offset is the global offset to the incidence angle θ and the dishing depth is the distance between the top of the SiCN layer and the top of the Cu layer. (b-d) Bayesian inference parameter estimations from a localized range (shown in axes) and sufficient sampling of 400,000 (200-by-200) in the 2D parameter space. (c) Reference marginal probability distribution for dishing depth d. Vertical lines correspond to 1, 2, and 3-sigma confidence intervals. Experimental conditions are set to be optimal for this sample according to [4]. (e-g) Bayesian inference parameter estimation with SMC sampler from a large initial range ($1\ nm \leq d \leq 4\ nm$ for dishing depth and $-1° \leq \Delta\theta \leq 1°$ for angle offset with 5000 samples.)

2. METHODS AND RESULTS

2.1 Efficient Bayesian Inference and Parameter Estimation

First, we demonstrate that a sequential Monte-Carlo sampler enables efficient and accurate calculation of the sample parameter posteriors that match more time-consuming reference results for a simulated copper interconnect sample (see Figure 1a).

In Bayesian statistics, given a forward model that predicts both signal y and corresponding noise from sample parameters θ, we can calculate a posterior distribution $p(\theta|y)$ that represents our belief of the sampler parameters given certain measurement y with

$$p(\theta|y) = \frac{p(y|\theta)}{p(y)} \cdot p(\theta). \qquad \text{(Eq. 1)}$$

In Equation 1, $p(y|\theta)$ represents the combination of our physical forward model and the noise model. It describes the likelihood of measuring y given certain sample parameters θ. Prior belief is represented by $p(\theta)$. For calculating the posterior distribution, the denominator $p(y)$ is simply a normalization factor as it is independent of θ. Bayesian inference can be seen as an intuitive method to perform parameter estimation given a physical forward model and noise. For EUV scatterometry, we have readily available physical forward models based on Fourier optics or rigorous EM solvers such as RCWA. We can also formulate the noise model from known detector parameters and photon statistics. [4]

However, calculating the posterior distribution in moderately high-dimensional parameters spaces can challenging. As the number of dimension increases, the number of samples required to finely sample the space becomes exponentially large. This curse of dimensionality can be addressed by Sequential Monte-Carlo (SMC) samplers, which employs an adaptive sampling strategy through annealing. [5]

Using an open source RCWA (RETICOLO [3]) model of the sample and a theoretical noise model for our instrument, we can compare a finely sampled (reference) posterior calculation to that by an SMC sampler. [3,4] For didactics, we consider a simple two-parameter case: the Cu interconnect recess depth and a global angle offset to the incident illumination, resulting in 2D posterior reconstructions. We first finely sample the 2D parameter space (200-by-200) and calculate the posterior distribution as well as its marginalized distributions in Figure 1b-d. On the other hand, Bayesian inference with a sequential Monte-Carlo sampler can reduce the computation time drastically and require fewer samples while still producing accurate posterior distributions (Figure 1e-g). The reduction in sampling size suggests that Bayesian inference in a moderately high-dimensional space is viable. We also note that the SMC sampler can locate and approximate a posterior that is extremely localized in the initial prior distribution.

2.2 Bayesian Adaptive Experiment Design on Buried Hf Grating

Efficient and accurate Bayesian inference via SMC can also calculate posteriors in a Bayesian Adaptive Experiment Design (BAED) framework for sequential EUV scatterometry measurements on a simulated buried Hf grating (schematic in Figure 2).

BAED is a statistical framework for sequential measurements where experimental designs are picked so that expected information gain (EIG) is maximized. It employs an iterative scheme where one starts with an initial belief of the sample parameter distribution, designs the next measurement based on the calculated EIG, make measurements, updates belief given the measurement, and repeats. [6]

Here, we propose an EUV scatterometry experiment on a 1D buried Hf grating consisting of 10 sequential designs, each repeated 5 times during the measurement process. The grating has two known layers of native silicon oxide and a known substrate of pure silicon. The parameters of interest are the thicknesses and densities of the amorphous silicon layer as well as the Hf grating structure underneath, along with a system calibration parameter describing a global offset to the angle-of-incidence.

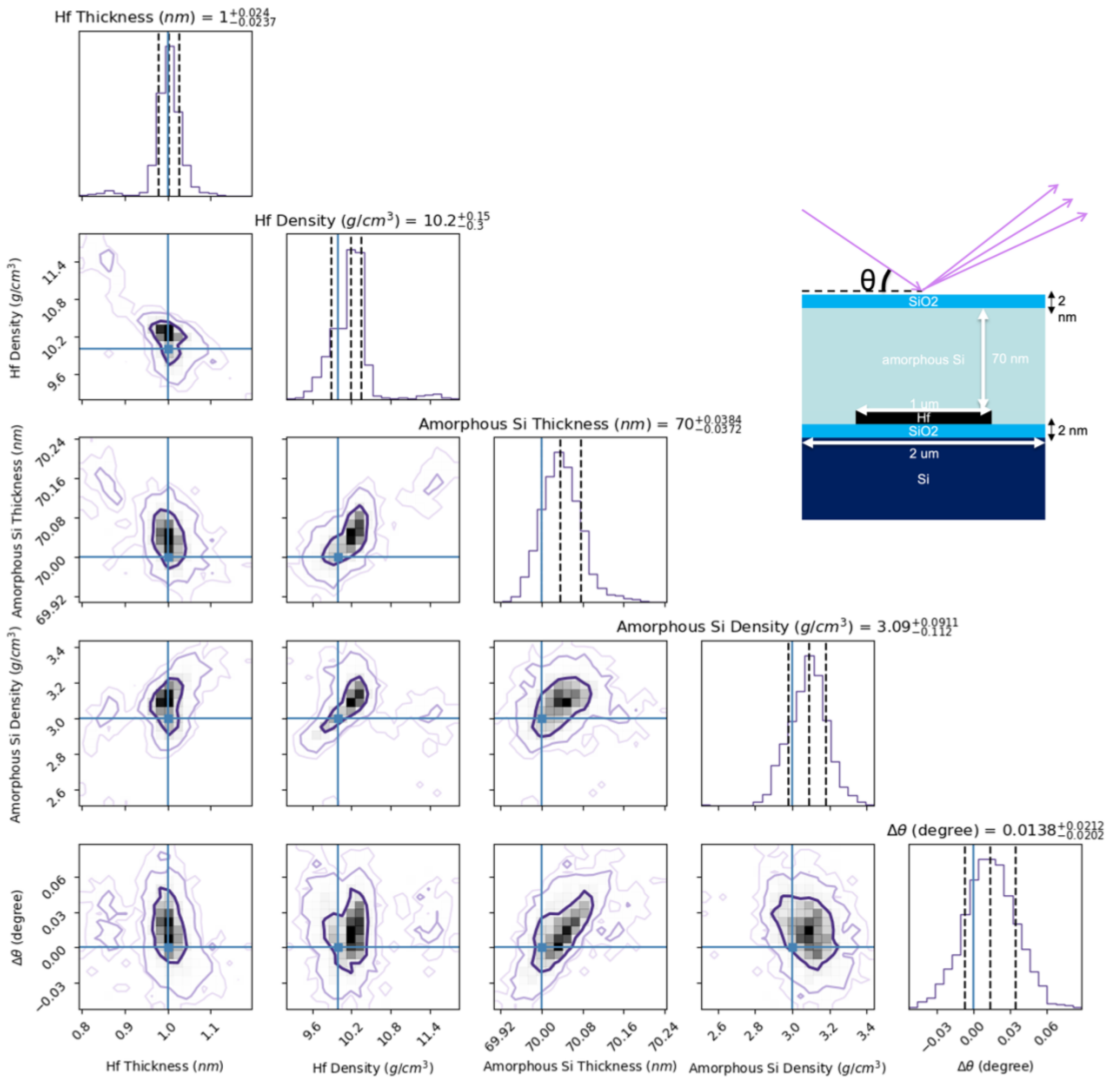

Figure 2, Results of proposed EUV scatterometry experiment on a buried Hf grating. Top right: simulated buried Hf grating schematic. From bottom left: corner plots of the five-dimensional posterior distribution after 50 total measurements (10 designs, each repeated 5 times) with 1-sigma, 2-sigma, and 3-sigma contours shown in varying shades of purple. Ground truth parameter values are shown in blue. In the marginalized distribution for single parameters, only the mean and 1-sigma (68%) intervals are plotted with dashed lines.

As shown in Figure 2 in the corner plots, we can achieve great sensitivity to the sample parameters, on the order of $0.1\ nm$ and $0.1\ g/cm^3$, after 50 total measurements. We note that, due to the limited number of repetitions at each designed measurement, there is bias evident in the marginal distributions. This is a practical consideration in implementing BAED as one trade speed for accuracy.

3. DISCUSSION AND CONCLUSION

This work demonstrates that EUV scatterometry can be reformulated as a closed-loop Bayesian experiment without prohibitive overhead. To reduce the additional runtime imposed by the inference and design phase of the BAED framework, we train a neural network to approximate the RCWA calculation in the physical forward model. The use of this surrogate model allows us to calculate the posterior and design the next measurement in under 10 minutes for the buried Hf grating, making the final implementation in an actual EUV scatterometry experiment viable. Note that the BAED framework also performs data analysis during data-taking, so the experiment concludes once the last inference is complete.

With the goal of implementing BAED EUV scatterometry measurements, we emphasize the importance of having an accurately calibrated noise model. Deviations within the distribution of measurements in the actual experiment translate to bias in the result.

In this study, we develop and validate the use of an SMC sampler in performing parameter estimation with Bayesian inference. With its efficiency and accuracy, we demonstrate end-to-end feasibility of an EUV scatterometry experiment with optimized sensitivity. Finally, we point out the fundamental importance of the noise model in this framework.

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4. REFERENCES

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