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Determination of an optimal measurement configuration in optical scatterometry using global sensitivity analysis

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ABSTRACT

In optical scatterometry, a proper measurement configuration has a significant impact on the precision of the reconstructed profile parameters beyond the quality of the measured signatures. In this paper, we propose to determine an optimal measurement configuration for optical scatterometry with the application of global sensitivity analysis (GSA). For each measurement configuration, we define a metric called the uncertainty index to evaluate the impact of random noise in measured signatures on measurement precision by combining the corresponding noise level with the main effect defined in GSA. Experiments performed on a one-dimensional silicon grating with its true dimensions close to its nominal values have revealed a trend that the lower the uncertainty index, the better the precision of the reconstructed profile parameters. This trend shows an agreement between the theoretically predicted and experimentally obtained optimal measurement configurations. The uncertainty index also predicts an optimal measurement configuration for a set of grating samples with various dimensions, which shows a similar trend in agreement with that by numerical simulations. In contrast, the optimal configuration predicted using the local sensitivity analysis method is significantly dependent on the nominal dimensions of the samples, and consequently it is difficult to achieve a proper configuration for all the investigated samples. The results suggest that the defined uncertainty index by the GSA method is suitable to determine an optimal measurement configuration, especially for a set of samples with relatively large dimensional variation.

1. Introduction

Recently, optical scatterometry has been widely used for critical dimension (CD) and overlay metrology in the semiconductor industry because it is fast, noncontact, nondestructive, and of low-cost compared to other techniques such as scanning electron microscopy (SEM) and atomic force microscopy [1–3]. As a model-based metrology, it involves both the forward modeling of sub-wavelength structures and the reconstruction of structural profiles from the measured signatures [4–6]; thus, it is a typical inverse problem with the objective of finding a modeled profile whose calculated signatures can best match the measured ones using regression analysis or library search [7,8]. Here, the general term 'signatures' contain the scattered light information from the diffractive grating structure, which can be in the form of reflectance, ellipsometric angles, Stokes vector elements, or Mueller matrix elements. The regression analysis or library search method optimizes a set of floating profile parameters (e.g., CD, side wall angle, and height) under a fixed measurement configuration, which is defined as a combination of selected wavelengths, incidence, and azimuthal angles [9]. In addition to the quality of the measured signatures, the measurement configuration also has a significant impact on the precision of the reconstructed profile parameters [10,11]. One method for improving precision is to enhance the quality of the instrument. Another method, also the focus of this research, is to determine an optimal measurement configuration that maximizes the sensitivity of the modeled signatures with respect to the variations of the profile parameters and at the same time minimizes the impact of the measurement noise on these reconstructed profile parameters.

Sensitivity analysis is a useful tool for qualitatively or quantitatively estimating the influence of the variations in model input profile parameters on the model output [12]. Currently, several approaches based on sensitivity analysis have been developed to determine an optimal measurement configuration for optical scatterometry. For example, Ku et al. conducted qualitative sensitivity analysis to select some feature regions containing all the possible incidence angles that yield the best sensitivity [13]. They proposed to reconstruct the profile parameters by seeking reflectance only in relatively few feature regions rather than in the full library, thus improving both the measurement precision and the measurement speed. Logofătu [14], Silver et al. [15], Foldyna et al. [16],

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and Germer et al. [17] performed statistical analysis to obtain the curvature matrix based on the partial derivatives of the modeled signatures with respect to the profile parameters over all the measurement configurations. The inverse of the curvature matrix is an estimate of the covariance matrix, and a minimization of the diagonal elements of the covariance matrix will optimize the measurement configuration for those corresponding profile parameters. Vagos et al. developed an uncertainty and sensitivity analysis package for guiding the model and azimuthal angle optimization processes [18]. In general, all the abovementioned approaches involve calculating the partial derivatives of the modeled signatures with respect to the profile parameters. This kind of partial derivative-based sensitivity analysis is usually called local sensitivity analysis (LSA), which examines the local response of the modeled signatures by varying one profile parameter by a small offset from its nominal value, while the others are fixed at their nominal values [19]. LSA has the advantage of being easy to conduct and is very efficient in reducing computational time. However, it cannot take into account the interactional influences among profile parameters on the model output and the local sensitivity index of a profile parameter is significantly affected by the fixed values of other parameters, when the model under analysis is non-linear.

In this paper, we propose to apply global sensitivity analysis (GSA) to determine an optimal measurement configuration that provides the best measurement precision in optical scatterometry. Under each measurement configuration, the two determining factors of measurement precision are the corresponding noise level of measured signatures and the sensitivities of the profile parameters. GSA is used to study how the uncertainty in the model output can be apportioned to different sources of uncertainty in the model input variables [20]. We introduce the global sensitivity measure (termed the main effect) to evaluate the individual influence of an input profile parameter on the forward model output. This sensitivity measure is obtained by floating all the input profile parameters of interest simultaneously and then looking at the entire input space rather than at a particular point in that space; it thus overcomes the fatal limitation of LSA when the model input parameters are uncertain and the model is of unknown nonlinearity. By combining the corresponding noise level with the calculated main effect, we define a metric called the uncertainty index to evaluate the impact of random noise in measured signatures on the measurement precision for each measurement configuration. A configuration with a minimum uncertainty index is expected to result in the best measurement precision. We use the uncertainty index to determine an optimal measurement configuration in optical scatterometry.

The remainder of this paper is organized as follows. Section 2 introduces our definition of the uncertainty index and illustrates its method of calculation in detail. Section 3 provides the predictions made by the calculated uncertainty index and its comparisons with experimental and simulated results. Finally, we draw some conclusions in Section 4.

2. Method

2.1. Definition of the uncertainty index

In optical scatterometry, the forward model can be mathematically abstracted as

$$y = f(\mathbf{x}, \mathbf{a}). \tag{1}$$

Here, $\mathbf{x} = [x_1, x_2, \ldots, x_n]$ is a vector representing a set of n input profile parameters (e.g., CD, side wall angle, and height); $\mathbf{a} = [\varphi, \theta, \lambda]$ represents a measurement configuration defined as a combination of azimuthal angle φ, incidence angle θ, and wavelength λ; and y denotes the model output under the measurement configuration $\mathbf{a}$. For any structure under measurement, the actual dimensions of profile parameters are always uncertain or have certain variations that deviate from their nominal values. Assuming that the profile parameters of interest follow some distributions which are uniform or normal, the global sensitivity stands for the global variability of the model output over the entire range of input profile parameters. The global sensitivity measures, which are formulated as conditional variances, are often classified as variance-based, and are usually evaluated by the Monte Carlo technique or by the Latin hypercube sampling process. Under a measurement configuration $\mathbf{a}$, the total variance of the model output $V_i(y, \mathbf{a})$ for the ith input profile parameter x_i is defined as [20]:

$$V_i(y, \mathbf{a}) = E\left[V_{\mathbf{x}_{\sim i}}(y|x_i, \mathbf{a})\right] + V\left[E_{\mathbf{x}_{\sim i}}(y|x_i, \mathbf{a})\right], \tag{2}$$

where $\mathbf{x}_{\sim i}$ denotes a vector containing all input profile parameters but x_i. The first term in the right side of Eq. (2) represents the expectation of the conditional variances and is usually called the residual, while the second term represents the variance of the conditional expectations and is called the main effect:

$$M_i(\mathbf{a}) = V\left[E_{\mathbf{x}_{\sim i}}(y|x_i, \mathbf{a})\right]. \tag{3}$$

Here, the meaning behind the inner expectation operator is that the mean of y is taken over all possible values of $\mathbf{x}_{\sim i}$ while keeping x_i fixed, and the outer variance is taken over all possible values of x_i.

As a global sensitivity measure, the main effect can be utilized to evaluate the individual influence of an input profile parameter on the model output. A large main effect implies that the variations of an input profile parameter have a significant influence on the uncertainty of model output while all the profile parameters are floating simultaneously, and, inversely, the variations in model output will have a small impact on the uncertainty of that profile parameter. Thus, the main effect is an important factor in determining how the random noise in measured signatures impacts the profile parameters during the reconstructing procedure. In addition, another main factor is the measurement noise level σ (standard deviation), which is usually different for each configuration. By combining the main effects of each input profile parameter and the corresponding noise level, we define a metric called the uncertainty index to evaluate the impact of random noise in measured signatures on the precision of each measurement configuration. The uncertainty index for the ith profile parameter under a given measurement configuration $\mathbf{a}$ is defined as:

$$U_i(\mathbf{a}) = \frac{\sigma(\mathbf{a})}{M_i(\mathbf{a})}. \tag{4}$$

In general, a measurement configuration with the minimum uncertainty index is considered optimal, and it would result in the best measurement precision.

2.2. Calculation of the uncertainty index

As the noise level is mainly dependent on the instrument used and is easy to obtain, the difficulty is in deciding how to calculate the main effect for each profile parameter under a given measurement configuration. Currently, a number of GSA techniques can be used to calculate this sensitivity measure, such as those suggested by Morris [21], Sobol [22], and the extended Fourier amplitude sensitivity test (EFAST) method [23]. Due to its robustness, especially for a small sample size, and its high computational efficiency, the EFAST method is adopted. Its core feature is a flexible sampling scheme over the multidimensional space of input profile parameters, which is specified by a set of transformation functions [23]:

$$\hat{x}_i(s) = \frac{1}{2} + \frac{1}{\pi}\arcsin[\sin(\omega_i s + \phi_i)], \tag{5}$$

where $\hat{x}_i(s)$ is the normalized x_i as a function of s in the range of [0, 1], s is a scalar variable varying over the range of $[-\pi, \pi]$, $\{\omega_i\}$ is a set of