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Efficient thin-film stack characterization using parametric sensitivity analysis for spectroscopic ellipsometry in semiconductor device fabrication

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ABSTRACT

During semiconductor device fabrication, control of the layer thicknesses is an important task for in-line metrology since the correct thickness values are essential for proper device performance. At the present time, ellipsometry is widely used for routine process monitoring and process improvement as well as characterization of various materials in the modern nanoelectronic manufacturing. The wide recognition of this technique is based on its non-invasive, non-intrusive and non-destructive nature, high measurement precision, accuracy and speed, and versatility to characterize practically all types of materials used in modern semiconductor industry (dielectrics, semiconductors, metals, polymers, etc.). However, it requires the use of one of the multi-parameter non-linear optimization methods due to its indirect nature. This fact creates a big challenge for analysis of multilayered structures since the number of simultaneously determined model parameters, for instance, thin film thicknesses and model variables related to film optical properties, should be restricted due to parameter cross-correlations. In this paper, we use parametric sensitivity analysis to evaluate the importance of various model parameters and to suggest their optimal search ranges. In this work, the method is applied practically for analysis of a few structures with up to five-layered film stack. It demonstrates an evidence-based improvement in accuracy of multilayered thin-film thickness measurements which suggests that the proposed approach can be useful for industrial applications.

1. Introduction

At present time, the accuracy and precision of the multilayered thin-film thickness measurements should match stricter requirements for routine process monitoring and control in the modern nanoelectronic manufacturing industry. Direct methods of characterization, such as various transmission electron microscopy (TEM) techniques [1], are inevitably destructive and time consuming, have very small sampling size and cannot be automated easily; therefore, those TEM-based methods are unusable for real-time in-line monitoring. Other well-established and non-destructive techniques, such as specular X-ray reflectometry [2–5], optical transmission/reflection spectrophotometric measurements, and multiangle spectrophotometry [6–9], allow characterization of multilayered thin film structures, although they require special efforts in order to get reliable information and exclude measurement errors (for instance, due to interfacial roughness [10] or unintentional presence of a few monolayers of surface contamination [11]). Among diverse characterization methods, one of the most convenient and well-established techniques to perform multilayered thin-film thickness measurements is spectroscopic ellipsometry (SE). Ellipsometry, in general, is an optical metrology technique which measures the changes in the polarization state of light upon reflection from a sample surface at non-normal (oblique) incidence and those changes typically expressed either in terms of two values (ellipsometric angles) called Psi (Ψ) and Delta (Δ) or a complex number ρ (complex reflectance ratio) (fundamentals of ellipsometry, instrumentations, data analysis as well as multiple applications are well described elsewhere [12–16]). SE involves measurements of Ψ and Δ as functions of wavelength λ (multi-wavelength approach) and, therefore, provides more information to determine the individual-layer thicknesses in complex multilayered structures. Also, SE combined with modern 2D and 3D scatterometry modeling is capable to monitor and control critical dimensions of the devices and other important structural parameters in a real production environment. Special note should be taken that ellipsometry is the *indirect* characterization method which requires appropriate modeling analysis and solution of an inverse problem, which is often ill-posed, using various multi-parameter non-linear global and local optimization algorithms [17–21]. Optical analysis compares the measured data with a suitable optical model in which a few parameters are allowed to vary to minimize the so-called *merit function* (or *error function*), i.e., the function which determines the quality of fit. This fact presents a significant challenge for unambiguous characterization of multilayered thin-film structures (like inter-layer dielectric (ILD) stack measurements [22] or very thick complex multilayered

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structures [23]) in semiconductor and optoelectronic devices processing since the number of simultaneously determined model parameters, for instance, thin film thicknesses and model variables that describe the film optical constants, should be small enough to greatly reduce or completely avoid cross-correlations between the fitting parameters. Many authors have reported about the challenges involving SE characterization of multilayered structures due to correlation concerns. For instance, thin silicon oxide–nitride–oxide (SiO_2–Si_3N_4–SiO_2, ONO) structure ellipsometric measurements without a deep-ultraviolet-extended spectral range are very affected by strong correlation between top and bottom oxide thicknesses [24,25]. Another well-known example of this issue includes correlation between thickness and optical constants of very thin absorbing films, such as metal or amorphous carbon films [26–28]. To overcome this issue and decorrelate the fitting parameters in characterization of multilayered thin-film structures or thin absorbing films, several methods based on complementary use of various optical techniques and their simultaneous analysis have been reported [24,28–35]. Those multi-technology methods allow significant reduction of parameter cross-correlations and, therefore, measurement uncertainties but are not available in most of industrial-grade optical metrology tools and also suffer from being significantly time consuming and impractical for routine in-line process monitoring.

Typically, the parameters of interest for high-volume semiconductor manufacturing are thin film thicknesses while the optical properties of the films can be determined separately. However, if the thin films in a complex multilayered stack have comparable optical properties for a selected spectral range (like in case of the ILD or ONO stacks) and, therefore, there is a quite limited contrast between the layers (low contrast imposes extra requirements on tool's calibration and signal-to-noise ratio), a strong correlation between, at least, some layer thicknesses generally occurs and differentiation of the film thicknesses can be a problem. In that case, compensation between film thicknesses can result in equally good quality of fit to the measured data across a wide range of thickness values and should lead to increased measurement uncertainties. Also, some layers might contribute less than others into the model simulation. Hence, the most essential/sensitive input model parameters need to be identified and ranked according to their significance for model outputs of interest. This problem of "sensitivity" is central to the understanding of the model behavior where the ill-defined parameters (for instance, cross-correlated parameters) will severely influence the accuracy of complex film stack characterization. A well-established way to quantify the parameters influence is to perform a sensitivity analysis (SA) [36,37]. It determines the relative importance of the parameters and helps to optimize a range of variations for each sensitive parameter since the efficiency of all optimization algorithms can be greatly improved if the parameter search space has reasonable bounds. In this way, it is more likely for optimization algorithm to find the unique global optimal solution rather than the multiple local minima which do not describe the results adequately. Another advantage is that it indicates which parameters have a negligible influence on model behavior and, therefore, might simplify the model and reduce the number of model parameters needed to be involved in the optical analysis. In spite of enormous occurrence of the SA methods in various disciplines, including unceasing discussions of SA for models with correlated parameters [38–42], there are a very few studies dealing with use of SA in different application areas related to optical metrology. For example, Ylilammi and Ranta-aho [6] performed quantitative sensitivity analysis by calculating the increase of the average misfit due to a small variation in the layer thickness and then computing the sensitivity of each layer. Recently, Gong et al. [43] modified the above-mentioned method by attempting to optimize also the ranges of thickness variations based on estimated layer sensitivities. Consequently, they suggested using wide search range for the thicknesses with low sensitivities while those with high sensitivities are searched in a more narrow range. However, this conclusion appears to be truly contrary to intuition and common sense. Indeed, for the parameter with low sensitivity the search in wide range of the parameter space might easily fall into one of the local minima after a few iterations and stay there without examining the surrounding areas. Also, such "sensitivity separation" method will be very difficult to implement in practice where there are spontaneous variations in layer thickness ("in-wafer" and/or "in-lot") due to alterations of the process conditions and the suggested way to estimate layer thickness range cannot be easily applied. Moreover, this differential analysis approach based on the first order Taylor series approximation investigates the impact of the parameters locally (so-called, local SA), i.e., the parameters are varied by a small amount from a baseline value. Thus, local SA is not able to assess full parameter influences unless some conditions for the model under study (such as, for instance, linearity) are fulfilled. Budai et al. [44] conducted sensitivity analysis of oscillator parameters used in the Tauc–Lorentz and Gaussian oscillator models by estimating the mean square error values near global minimum. Another approach to sensitivity analysis of oscillator parameters in the Tauc–Lorentz model has been discussed in Ref. [45] in the context of optical scatterometry modeling. Foldyna et al. [46] performed sensitivity calculations based on virtual experiments to estimate an optimal measurement configuration in optical scatterometry. In the paper by Dong et al. [47] another methodology to determine optimal measurement configuration within the framework of the global sensitivity analysis was developed.

The present study is devoted to the development of a systematic and practical approach to determine the relative importance of various model factors influencing an accuracy of multilayered thin-film thickness measurements. A practical method is proposed, based on parameter ranking, to establish optimal bounds on the parametric search ranges which allow more likely to avoid wrong solutions in multilayered thin-film characterization. The practical application of this method is demonstrated by two examples of complex thin-film structure characterization.

2. An approach to parametric sensitivity analysis

To identify and prioritize the most influential model parameters, the sensitivity of the optical model to those parameters needs to be tested. There is a wide assortment of analytical and numerical methods to perform the sensitivity analysis, some of which are quite simple and practical, i.e., easy to implement. In the literature, the most popular SA technique is based on the so-called "one-at-a-time" or "one-factor-at-a-time" (OAT/OFAT) approach: sensitivity may be estimated by calculating changes in the model's output when varying one selected parameter at a time by small amount from its baseline (or "nominal") value while holding all other parameters fixed at their nominal values. The main disadvantages of the OAT/OFAT methods are that they 1) use a very restricted range of the input parameter variations and 2) assume an independence of the parameters. However, in many practical cases the input parameters are correlated with each other and varying one input parameter at a time while holding others fixed may produce some false SA results (see, for example, Ref. [48] for a well-reasoned critique of the OAT/OFAT approaches). Here we implement a screening-type technique based on so-called "elementary effects" (EEs) method (or method of Morris) [49]. The EEs method uses two sensitivity measures for each input parameter: the index μ (or μ^* in revised Morris method [50]), which estimates the overall importance of the parameter, and the index σ, which describes non-linear effect on model's output and/or interactions with other input parameters. For each input parameter an *elementary effect* (EE_i) is defined as:

$$EE_i = \frac{Y(X_1, X_2, \ldots, X_{i-1}, X_i + \Delta_i, \ldots, X_k) - Y(X_1, X_2, \ldots, X_k)}{\Delta_i}, \quad (1)$$

where Y is the model output of interest (for instance, the merit function as a measure of the agreement between data and the fitting model), and X_i, $i = 1, \ldots, k$, is the ith model (input) parameter. r elementary effects