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A practical method for optical dispersion model selection and parameters variations in scatterometry analysis with variable *n*&*k*'s

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ABSTRACT

Optical critical dimension (OCD) scatterometry in recent years became a well-accepted and powerful technique to determine the properties and grating profiles of 2D and 3D microelectronic structures (critical dimensions, side-wall angles, grating and underlying thin film thicknesses) in modern semiconductor manufacturing. However, the optical scatterometry, as any model-based metrology technique, relies on the accuracy of the OCD model which highly depends on the optical properties (the *n*&*k*'s) of the materials in the structure. In practice, even small deviations in material's optical properties (from nominal model inputs) due to process condition variations might significantly affect the scatterometry measurements. A logical way to deal with this problem is to allow some degree of the *n*&*k*'s variability of the most affected layer(s) in the OCD model describable by relevant dispersion model(s) (floating *n*&*k*'s). Essentially, one of the largest complications for the end users (process engineers) is to decide which optical dispersion model (Cauchy, Lorentz, Tauc–Lorentz, etc.) needs to be selected to describe a material under production conditions and which parameters are more sensitive and need to be floated in the OCD model. We developed an approach which, we believe, will result in more straightforward and fast development of the OCD models. This approach provides a possibility to automatically select a most proper dispersion model which has been always an ambiguous decision for most of the end users. This methodology will allow determination of most influential model parameters to vary, eliminating potential sources of modeling error at the initial steps of the OCD modeling. A few examples to illustrate the key ideas and practical use of our procedure have been provided.

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1. Introduction

Nowadays, optical critical dimension (OCD) metrology (a.k.a., "scatterometry") is a widely-used in-line optical technique in semiconductor volume manufacturing to control the process ranges of 2D and 3D microelectronic structures, namely, critical dimensions, side-wall angles, grating and underlying thin film thicknesses, since those properties directly influence device performance [1–4]. Currently, this technology is based on spectroscopic or angular configurations with different measurement methods – ellipsometry, reflectometry (polarized or unpolarized) or their combination. OCD metrology has the advantages to be fast, non-intrusive, non-invasive, non-destructive and informative measurement technique which does not require special sample preparations. In general, the sample is unaltered and the measurement itself does not cause any damage since OCD tools use relatively weak light sources. However, we should bear in mind that OCD is the *indirect* characterization method which requires appropriate modeling analysis depending on the nature of monitored or controlled processes to achieve accurate and reliable results. Scatterometric analysis compares the measured data with suitable optical model using the rigorous coupled-wave analysis [5]. And, as a model-based metrology technique, it relies on the accuracy of the optical model which highly depends on the optical properties (the optical constants [*n*&*k*] or the complex dielectric function ε) [6] of the materials in the structure. In traditional approach the *n*&*k*'s of the films in the stack are considered as fixed inputs in the OCD model. On the one hand, this assumption may seem natural and advantageous since it does not overcomplicate the OCD model. However, in practice, even relatively small deviations in material's optical properties (from nominal model inputs) due to process condition variations may significantly affect the scatterometry measurements [7]. A logical way to deal with this problem is to allow some degree of the *n*&*k*'s variability of the most affected layer(s) in the OCD model describable by relevant dispersion model(s) (floating *n*&*k*'s). A few articles have been published recently which use the "floating *n*&*k*'s" approach and demonstrate an undoubted necessity of taking into account the *n*&*k*'s variability to achieve required accuracy of the scatterometry measurements [8–12]. The recently developed "scatterometric porosimetry" [13,14] combines the ellipsometric porosimetry with scatterometric technique and includes the refractive index modeling to characterize the plasma-induced modifications in porous low-*k* dielectrics on patterned structures. Of course, as a drawback of this approach we get more floating parameters in the OCD

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Table 1
Parameter values in the Cauchy–Urbach dispersion model (2), (3) for initial simulated families of the lower and upper bounds *n*&*k*'s.

Model parameter	Dataset I	Dataset II
A_n	1.45 and 1.50	1.45 and 1.50
B_n	0.01	0.01 and 0.03
C_n	0	0
A_k	0.001	0.001 and 0.005
B_k	1.3	1.3 and 1.6
λ_0	400	400

model and possibility of strong cross-correlations between the model parameters which may, potentially, lead to some ambiguity in interpretation of scatterometry measurements and higher measurement uncertainties. To militate against the impact, it is necessary to intelligently decide, for a given application, which parameters need to be floated or fixed. Alternatively, in order to overcome the *n*&*k*'s variability issue, Vaid et al. [15,16] suggested the complementary use of multiple targets which might increase the amount of useful information added to the OCD model and reduce parameter cross-correlations lowering thereby the measurement uncertainties. Unfortunately, this multi-target methodology will drastically reduce throughput performance of metrology tools and, therefore, increase the number of optical metrology tools required per fabrication facility.

Most of the modern commercial scatterometry software packages for OCD modeling, such as TeraGen ODP™ (version 2008, Timbre Technologies, Inc., a wholly owned subsidiary of Tokyo Electron Limited (TEL), Santa Clara, CA, U.S.A.), AcuShape™ (version 2, jointly developed by Timbre Technologies, Inc., a wholly owned subsidiary of Tokyo Electron Limited (TEL), Santa Clara, CA, U.S.A. and KLA-Tencor Corporation, Milpitas, CA, U.S.A.), NovaMARS® (version 5, Nova Measuring Instruments Ltd., Rehovot, Israel), NanoDiffract™ (version 3, Nanometrics, Inc., Milpitas, CA, U.S.A.), include "floating *n*&*k*'s" option to account for influence of *n*&*k* variations. Essentially, one of the largest complications for the end users (process engineers) is to decide which optical dispersion model (Cauchy, Lorentz, Gaussian, Tauc–Lorentz, etc.), that is used to describe the variations in the optical properties of the materials, needs to be selected to characterize a material under production conditions and which parameters are more influential and need to be floated in the scatterometric model. If too many parameters are allowed to vary, the further optimization process can become numerically unstable and evidently some model parameters have to be fixed. In this paper we developed an approach which, we believe, will result in more straightforward and fast development of the OCD models. This approach provides a possibility to automatically select most proper dispersion model which has been always an ambiguous decision for most of the end users. This methodology will allow a determination of correct material optical model and most significant model parameters to vary eliminating potential sources of modeling error at initial steps of the OCD modeling. The "floating *n*&*k*'s" function could be optimized to exclude complicated (and time-consuming) analysis of dispersion model selection and need for expertise from high-level metrology specialists. By automation of such complicated optical model selection, some usual modeling ambiguities can be eliminated and such solution will be more attractive to process engineers and end users than a common "*n*&*k*'s extraction and analysis" approach.

2. Description of the methodology

We propose the following: (i) To build a family of possible material's optical properties as a function of wavelength λ (or photon energy $E = hc/\lambda$, where h is the Planck constant and c is the speed of light) relying on known optical constants and using one of the effective medium approximation (EMA) mathematical expressions [17–21] to mix the *n*&*k*'s and create multiple intermediate dispersions. (ii) To perform non-linear curve fitting for all *n*&*k* dispersions from the "sample set" of dispersions. (iii) To report to a user which parameter(s) has(have) strongest influence to obtain a good simultaneous fit for all *n*&*k*'s from the "sample set" family. In general, it should also provide users with justified and accurate recommendation for preferable dispersion model for a given material, based solely on intelligent correlation analysis and best curve-fitting criteria.

Formally, to fully realize those intentions, the following steps are required:

1. To start the procedure we need two initial *n*&*k* dispersions for the material under study which represent high and low bounds on the observed variations of the optical properties in production line (as an example, we can consider a thin film produced by different deposition tools). An alternative way is to implement some known process variations (say, $\pm 5\%$) which will be representative of real production conditions.
2. Then we need to create a set of intermediate *n*&*k* dispersions by mixing the dispersions of the constituents. Therefore, the process variations are treated as a continuous set of dispersion curves parameterized by the volume fractions of the components [22,23]. It is well-known that the composite dielectric function of a mixture of two or more material can be approximated by using one of the choices of the effective medium approximation. In the present study, the widely accepted self-consistent Bruggeman EMA (BEMA) [17–21] is used for generation of the family of intermediate *n*&*k* dispersions

$$f_{\mathrm{a}}\frac{\varepsilon_{\mathrm{a}}(\omega)-\varepsilon_{\mathrm{eff}}(\omega)}{\varepsilon_{\mathrm{a}}(\omega)+2\varepsilon_{\mathrm{eff}}(\omega)}+f_{\mathrm{b}}\frac{\varepsilon_{\mathrm{b}}(\omega)-\varepsilon_{\mathrm{eff}}(\omega)}{\varepsilon_{\mathrm{b}}(\omega)+2\varepsilon_{\mathrm{eff}}(\omega)}=0, \quad (1)$$

where a and b denote the two constituents (it can be generalized for more than two components [29–31]) with different complex dielectric functions (ε_{a}, ε_{b}) and volume fractions f_{a} and $f_{\mathrm{b}} = (1 - f_{\mathrm{a}})$, respectively, $\varepsilon_{\mathrm{eff}}$ is the dielectric function of the mixture, and $\omega = 2\pi c/\lambda$, c is the speed of light. Thus, we obtain a "sample set" of dispersions which represent possible *n*&*k* variations under production conditions.

3. The procedure then can select one of the "built-in" dispersion models or, in simplified version, request for user's input regarding dispersion model selection and initial values of the model parameters.

Table 2
Parameter values obtained by non-linear optimization procedure with the Cauchy–Urbach dispersion model for the 1st family of simulated *n*&*k* spectra.

Model parameter	Subset 1 (0%)	Subset 2 (20%)	Subset 3 (40%)	Subset 4 (60%)	Subset 5 (80%)	Subset 6 (100%)
A_n	1.450000	1.459952	1.469926	1.479926	1.489950	1.500000
B_n	0.010000	0.010000	0.010000	0.010001	0.010000	0.010000
C_n	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
A_k	0.001000	0.001000	0.001000	0.001000	0.001000	0.001000
B_k	1.300023	1.300020	1.300019	1.300019	1.300020	1.300023
λ_0	400	400	400	400	400	400

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