A new method to derive best-fit parameters and their uncertainties from depolarizing Mueller-matrices

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The non-optimal treatment of depolarization in current approaches to evaluate Mueller matrix measurements may lead to systematic measurement errors and inadequate uncertainty estimations. We developed a novel method to derive best-fitting sample parameters and reliable corresponding uncertainties from measured Mueller matrices in a physically reasonable way.

1 Introduction

Spectroscopic ellipsometry is a versatile tool to measure dimensional or optical parameters of surface layers or structures. For determining the parameters, the solution of an inverse problem is needed. It is achieved by a fitting procedure, which compares simulated to measured quantities within a merit function to be optimized.

Our goal is to attain reliable and traceable Mueller matrix (MM) ellipsometry for dimensional nanometrology. To realize that, a full uncertainty consideration is necessary.

Providing realistic measurement uncertainties, hardware, measurement and analysis induced uncertainty contributions have to be regarded. Here we focus on the last two aspects.

2 New optimization method

In order to consider these uncertainty contributions first it was necessary to treat depolarization and measurement noise in a reasonable way. Commonly used merit functions treat depolarization as a residual error in the optimization process and the best-fit solution has the smallest overall one. Instead, we use depolarization to derive a weighting for our merit function and do not treat it as an object to be minimized. In this way we ensure to treat depolarization as an optical property (e.g. through roughness of surface) and after some computation ([2]) we end up first in the new merit function

$$\sum_{\lambda}^{N} \boldsymbol{j}_{s,\lambda}^{\dagger} \boldsymbol{H}_{m,\lambda}^{-1} \boldsymbol{j}_{s,\lambda} \qquad (1)$$

with the measured Cloude covariance matrix $\boldsymbol{H}_m$ ([1]) and the simulated Jones-element vector $\boldsymbol{j}_s$.

Including also measurement noise in the new optimization method we extended (1). To that purpose we exploit raw data provided by our Sentech SE 850 ellipsometer (Fig. 4) and get not only the best-fit MM-element vector $\boldsymbol{m}$ but also its covariance matrix $\boldsymbol{\Sigma}_m$ which is propagated then to $\boldsymbol{H}_m$. At the end there is a so-called Cloude-filtered matrix $\boldsymbol{H}_{CF}$ in the merit function (instead of $\boldsymbol{H}_m$), which is calculated from the mean filtered MM. Further details of the new optimization method will be published soon.

3 Application on simulated data

To ensure the operability of our new merit function, we first tested it for simulated data of an SiO_2-Si layer model (Fig. 1). To get data containing depolarization, MMs (for an angle of incidence of 70°) were calculated for a large number of Gaussian distributed SiO_2 layers (mean: 2 nm, standard deviation: 0.1 nm). The mean of all calculated MMs gives a depolarizing MM. The new merit function returned exactly the preset standard deviation of 0.1 nm. In contrast, common merit functions result in extremely small and wrong uncertainties (e.g. 0.0002 nm). In the next step we tested the new merit function for noisy MM data with different uncorrelated noise levels and 3 different SiO_2 layer thicknesses (2 nm, 50 nm, 100 nm). With increasing noise level the uncertainty of the SiO_2 thickness increases (Fig. 2).

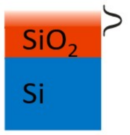

Fig. 1 *Simulated model*

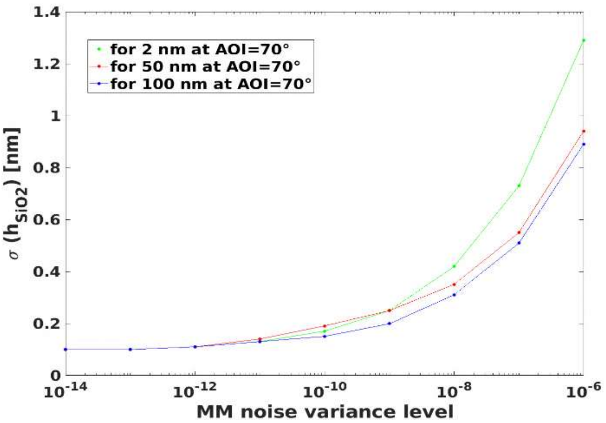

Fig. 2 *Simulated layer thickness uncertainties vs. MM noise variance levels for different SiO_2 thicknesses*

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For typical experimental MM noise variances of about 10^{-9} to 10^{-10} a slightly increased uncertainty is expected. This behaviour is confirmed by a corresponding Bayes analysis, see Fig. 3, which shows for a 2 nm layer thickness an approximately Gaussian posterior layer thickness distribution.

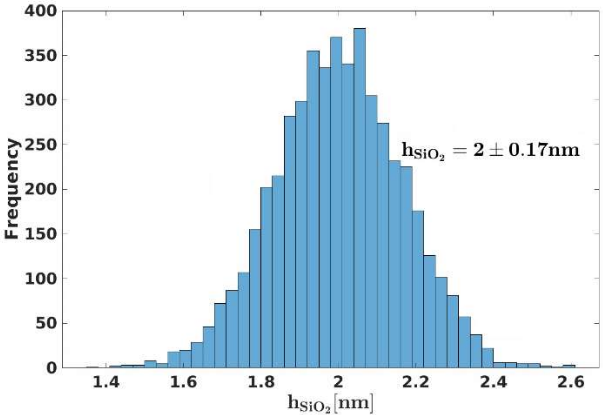

***Fig. 3** Posterior layer thickness distribution for a 2 nm SiO_2 layer thickness (Bayes analysis for a MM noise variance level of 10^{-10})*

4 Application on measured data

For the application on real data we used measurement data obtained on Si wafers with ellipsometers from Sentech (Fig. 4).

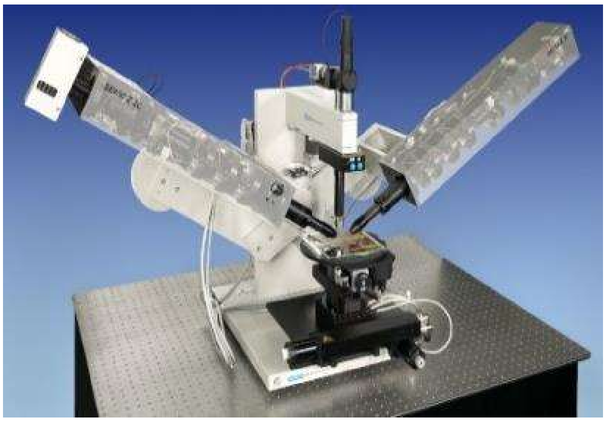

***Fig. 4** Sentech SE 850 spectroscopic Mueller ellipsometer to measure the full Mueller matrix*

Dispersion data	Model 1 [4]	Model 2 [3]
h_{SiO2}[nm] (mean val.)	1.80	2.19
σ [nm]	0.70	0.85
χ^2 (opt.:1)	1.15	1.13
BIC (Model 1 = 0)	0	-201

***Tab. 1** SiO_2 layer thickness data obtained using two different dispersion data.*

Since the new merit function can also be extended to a likelihood function, it enables the use of the Bayesian information criterion (BIC). Tab. 1 shows the result of this analysis using an SiO_2-Si model as in Fig. 1 for two different dispersion data sets. Model 2 leads to a smaller BIC value and is thus the better model (also yielding a smaller χ^2value). Please note that the better model according to the Bayes information criterion yields in this case a larger uncertainty for the layer thickness. The corresponding posterior layer thickness distribution is shown in (Fig. 5).

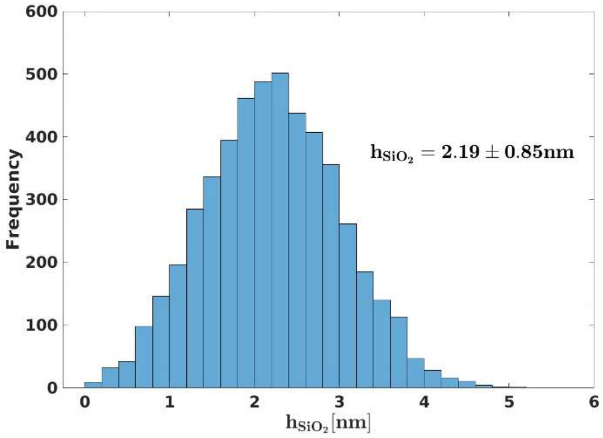

***Fig. 5** Posterior distribution for the SiO_2 layer thickness for Model 2 of Table 1. The distribution is approximately Gaussian and in good agreement with the according maximum-likelihood results.*

5 Summary and Outlook

The presented application examples confirm that the new optimization method takes depolarization and measurement noise correctly into account and yields plausible results. Furthermore, it turns out, that the now obtainable Bayesian information criterion is a suitable tool for judging different models. The next steps will be further tests on layer thickness standards and laterally structured samples. In addition, the method will be extended to include the influence of hardware parameters.

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