Bayesian approach for determining the optical constants of layered systems using EUV reflectometry: The effect of different priors.

O. Henze[1], V. Soltwisch[1], A. Tiwari[2], I.A. Makhotkin[2], N. Hegemann[1] and S. Heidenreich[1]
[1]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany
[2]University Twente, MESA Inst Nanotechnol, Ind Focus Grp XUV Opt, Enschede, Netherlands

For the development of novel technologies and high-precision manufacturing techniques in semiconductor and optics industries and in nanotechnologies, precise knowledge of the optical properties of these materials is vital, providing the foundation e.g. for novel nanoelectronic devices, high-quality sensors or effective photovoltaic elements.

The accurate measurement of optical properties in the extreme ultraviolet (EUV) spectral range around 13.5 nm remains a challenge for the development of optical components like photomasks, mirrors or gratings. Effects caused by surface roughness or oxidation can significantly influence the optical response of the systems in the EUV range. One method for measuring optical constants (n&k values) in the EUV range involves direct absorption measurements by transmission through thin free-standing films. However, it is often not guaranteed that the optical constants measured in this way can be directly transferred to complex multilayer systems. The determination of optical constants from reflectance measurements of systems that are very close to the actual target design of the mirror or multilayer system is significantly more complex, but also allows more information to be derived. In reflectometry, an inverse problem needs to be solved to obtain the parameter of interest. This inverse problem in optical metrology is frequently ill-posed, making the reconstruction of a complex layer system from a singular EUV reflectometry measurement typically unfeasible. The simultaneous determination of layer thicknesses, roughness and optical constants requires an increase in information density. This can be achieved by scanning the reciprocal space in which the incident wavelength is varied during the reflectometry measurements. The Bayesian approach is often used to derive optical constants, geometry parameters and associated uncertainties from reflectometry measurements. While this method offers many advantages, such as regularisation, a major drawback is the ambiguity of the choice of priority distribution. Our study addresses the effects of choosing different priors on the measurement results.

Experimental Part

The experiments were conducted in the Physikalisch-Technische Bundesanstalt (PTB) laboratory at the electron storage ring BESSY II at PTB's soft X-ray beamline, which covers the photon energy range from 50 eV to 1800 eV. The SX700 monochromator of the beamline provides a spectral resolution below 0.25 eV. To suppress higher orders, different foil filters (C, B, Be, Si, and Al) have been used, depending on the spectral range. The reflectometry experiments can be described as follows: a monochromatic beam with the photon energy h impinges on the sample surface at a variable angle of incidence (aoi). The elastically scattered wave propagates along the exit angle, where the specular reflectance (=) from the sample is measured in -polarization with a GaAsP photodiode. A lubricant-free goniometer inside the vacuum chamber allows for precise rotation and positioning of the samples, aligning the angle of incidence with an uncertainty below ±0.01° with respect to the incoming beam. In this study a single Ruthenium layer on a Silicon substrate was considered. The Ru layer sample was fabricated with magnetron sputtering at the Mesa+ Institute at the University of Twente on a silicon substrate, with a nominal layer thickness of 30 nm.

Inverse problem: Bayesian Approach

The Bayesian approach is well suited to solve the inverse problem of reflectometry since it determines not only the parameters of interest (optical constants, layer thickness, layer roughness), but also provides a scheme for regularization by prior knowledge. However, the results could be affected by the choice of the prior. In the study reported here the sensitivity of the Bayesian approach to EUV-reflectometry for thin layer systems with respect to the choice of different priors was investigated numerically. Following [1,2], the basis for the approach is the Bayes' theorem:

$$\pi(\mathbf{p}, a; \mathbf{y}) = \frac{\mathcal{L}(\mathbf{p}, a; \mathbf{y})}{\int \mathcal{L}(\mathbf{p}, a; \mathbf{y})\pi_0(\mathbf{p}, a)}\pi_0(\mathbf{p}, a).$$

Here **p** are the parameters of interest (layer thickness, roughness and optical constants of the layers), and 'a' is a hyperparameter (parameter modelling the measurement error). π_0 is the prior distribution that encodes prior knowledge about the parameter of interest. The posterior distribution π is a multivariate distribution of parameters of interest and the function L(**p**, a; **y**) is the likelihood given by

$$\mathcal{L}(\mathbf{p}, a; \mathbf{y}) = \Pi_{j=1}^{m}(\sqrt{2\pi}\sigma_j(\mathbf{p}, a))^{-1} \exp\left[\frac{(f_j(\mathbf{p}) - y_j)^2}{2\sigma_j(\mathbf{p}, a)^2}\right],$$

where the parameter 'a' is determined by the error model [3] σ_j(**p**, a) = a · f(**p**) and f(**p**) is given by the forward model describing the reflection on the layered system. As a forward model, we used the Transfer-matrix-method including surface roughness [4]. In order to estimate the parameter of interest, i.e., to calculate the posterior distribution by Markov Chain Monte Carlo (MCMC) sampling methods, a prior distribution π_0 has to be chosen. The choice of the prior distributions may affect the resulting posterior distribution and thus the results of the indirect measurement. To investigate the effect of the priors on the reconstruction results, different priors were chosen for the error parameter 'a' (see table 1) and the posterior distribution was calculated using MCMC sampling for reflectometry measurement data y_j. Here, the index 'j' indicates the different wavelengths (10 nm to 20 nm, 1nm steps).

Table 1: Choice of prior distribution for different parameters. Priors for n&k are chosen as uniform distributions with -10% of the value of the refractive index table [5] for Si and Ru for the lower bound and +10% of this value for the upper bound.

parameter	prior distribution
RU thickness	U[27,36](nm)
RU roughness	U[0.0,2.0](nm)
Si roughness	U[0.0,1.5](nm)
a (error setup 1)	U[0.01,0.1]
a (error setup 2)	U[0.01,0.25]
a (error setup 3)	U[0.05,0.2]
a (error setup 4)	U[0.05,0.1]

Results

Following Vignaud et al. [6] a Transfer-matrix-method was implemented that incorporates the surface roughness into the forward model to model the reflectometry measurements. Based on this forward model a Python script with the EMCEE algorithm [7] was used for MCMC samplings. In particular 64 walkers and chain lengths of 400.000 steps has been chosen. The burn in phase was about 20.000 steps. Fig. 1 shows the marginals of the posterior distribution for parameter pairs. The posterior is similar to a multivariate Gaussian distribution with certain correlations. From each posterior distribution we calculated the n&k values, layer thickness and roughness of Ru, roughness for Si and the error parameter 'a' for the different wavelengths.

Fig. 2a shows a comparison between the marginals of the posterior distributions for the optical constant 'n' for different prior distributions of the error parameter 'a' (wavelength of the incident light was 11 nm). It can be clearly seen that the mean values of the distributions do not differ, but the standard deviation of n is slightly different. The connection between the chosen prior distribution and this trend is not obvious since the error parameter 'a' is determined simultaneously for all wavelengths. Fig. 2c-d. shows the mean values of the posterior for n&k optical constants for wavelengths of the incoming beam of 10nm to 20nm. Except for the outliers at the wavelengths 10 and 12 nm, the mean values of the n&k values collapse to form a curve. A closer look at the 10 and 12 nm cases shows that there seem to be multimodal posterior distributions. Since our chosen MCMC sampler has some difficulty sampling multimodal distributions, the results depend on the initial configuration and further investigation is needed. The reason for the occurrence of multimodal n&k values could be the vicinity to the Si-L2,3 absorption edge.

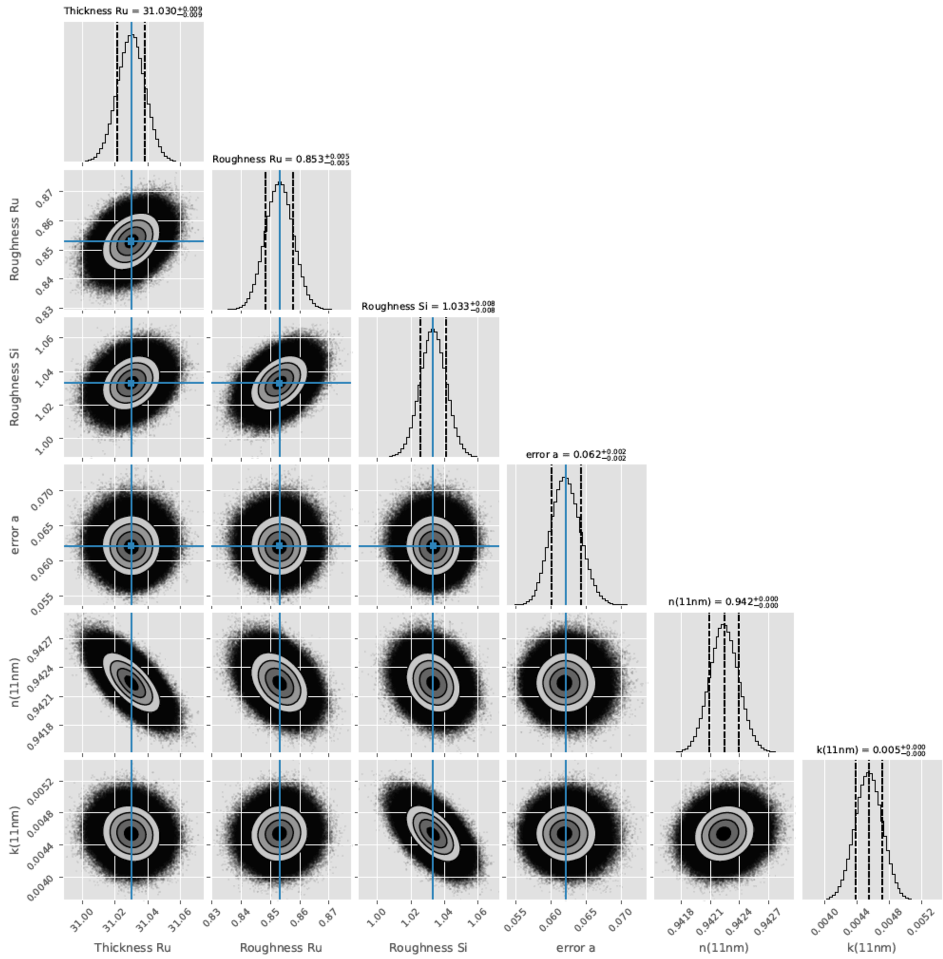

Figure 1: Posterior distribution depicted as marginals of parameter pairs.

In contrast to the mean values, there are slight differences in the standard deviation, which increase with increasing wavelength (see Fig. 1e-f). If one compares the simulated reflectivity for the determined mean values for n&k with the measured reflectivity, one obtains a very good agreement, also for the outliers (Fig. 1b).

Conclusion

Bayesian inversion is a powerful tool to determine the measurand for indirect measurements and its associated uncertainties. However, the choice of the prior may have an effect onto the results. In the proceeding we have shown for a specific layer sample, the determined optical constants (mean values of the posterior) are robust against variations of the prior distribution for the error parameter ‘a’. However associated uncertainties are affected. With increasing wavelengths of the incident light, deviations of the uncertainties of the optical constants determined for different priors increases. This work was carried out as part of an initiative to determine the optical constants of layer systems. Further results can be found here under the following URLs [8].

Acknowledgement

This work was supported by the project 20IND04 ATMOC. This project (20IND04 ATMOC) has received funding from the EMPIR programme co-financed by the Participating States and from the European Union’s Horizon 2020 research and innovation programme.

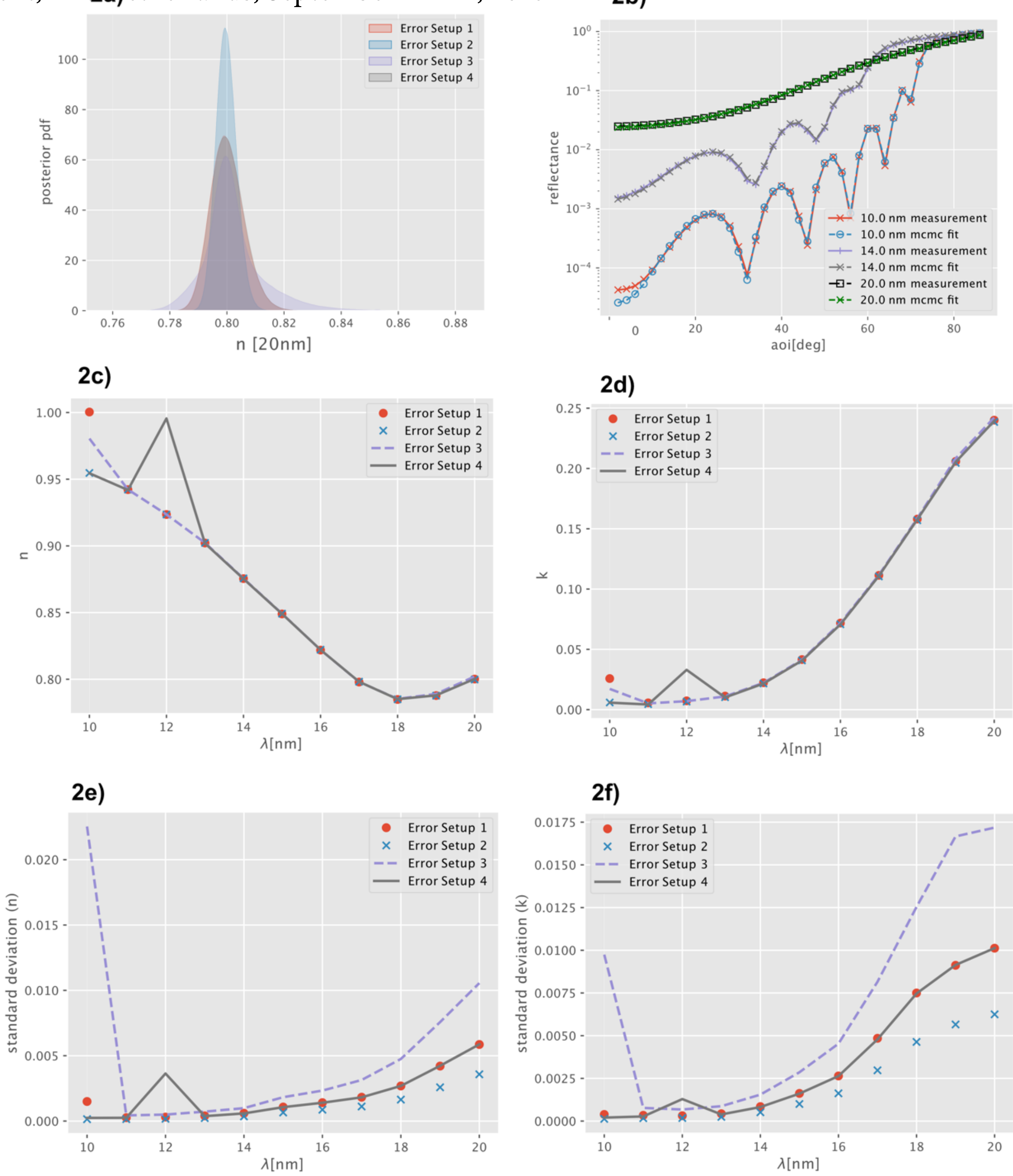

Figure 2: a) Distribution for ‘n’ at wavelength 20 nm for different prior distributions for the error parameter ‘a’. 2b) Comparison of the fit with experimental reflectance data for selected wavelengths. 2c-d) Dependence of the median of n&k values on the wavelengths for different priors of the error parameter ‘a’. 2e-f) Dependence of the standard deviation of n&k values on the wavelengths for different priors of the error parameter ‘a’.

[1] Heidenreich S, Gross H, Bär M, Bayesian approach to determine critical dimensions from scatterometric measurements, Metrologia 2018, 55 (6), S201.

[2] Heidenreich S, Gross H, Bär M, Bayesian approach to the statistical inverse problem of scatterometry: Comparison of three surrogate models, Int. J. Uncert. Qunatification 2015,5(6), 511.

[3] Farchmin N, Hammerschmidt M, Schneider P-I, Wurm M, Bodermann B, Bär M, Heidenreich S, Efficient Bayesian inversion for shape reconstruction of lithography masks, J. Micro and Nanolith. MEMS and MOEMS 2020, 19 (2). 204001.

[4] Ciesielski, R., Saadeh, Q., Philipsen, V., Opsomer, K., Soulié, J., Wu, M., Naujok, P., van de Kruijs, R., Detavernier, C., Kolbe, M., Scholze, F., & Soltwisch, V. (2021). "Determination of optical constants of thin films in the EUV".

[5] B.L. Henke, E.M. Gullikson, and J.C. Davis. X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30000 eV, Z=1-92, Atomic Data and Nuclear Data Tables Vol. 54 (no.2), 181-342 (July 1993).

[6] G. Vignaud and A. Gibaud, “REFLEX: a program for the analysis of specular X-ray and neutron reflectivity data,” J. Appl. Crystallogr., vol. 52, no. 1, pp. 201–213, 2019.

[7] J. Goodman and J. Weare, Ensemble samplers with affine invariance, Communications in Applied Mathematics and Computational Science., 5 (2010).

[8] https://www.ocdb.ptb.de, https://www.atmoc.ptb.de/home/