USE OF P-SPLINES FOR THE DIELECTRIC FUNCTION REPRESENTATION IN THE INTERPRETATION OF SPECTROSCOPIC ELLIPSOMETRY DATA

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About ten years ago Johs and Hale developed the Kramers–Kronig consistent B-spline formulation for the dielectric function modeling in spectroscopic ellipsometry data analysis [1]. But the actual performance of B-spline parameterization strongly depends on the number of knots (and, in general, their locations) used to describe the dielectric function. It is intuitively easy to conceive that fewer knots in the considered wavelength range may not be enough to fit all essential spectral features (underfitting). On the contrary, increasing the number of knots beyond the optimal value can result in significant overfitting of the experimental data, i.e., leads to an unrealistic result with measured noise reproduction. In previous papers [2,3], we used well-established information criteria approach for choosing a suitable B-spline model with optimal number of knots to balance fidelity to the measured data and complexity of the fit.

An alternative method to avoid overfitting by B-spline parameterization is to use one of the variants of smoothing splines called “penalized splines” or “P-splines” which include a penalty on B-spline coefficients. The amount of penalty, which based on the second- (or higher-) order finite differences of the coefficients of adjacent B-splines, is easily controlled by non-negative smoothing (or penalty) parameter α. Selection of $\alpha = 0$ leads to ordinary least-squares fit of the ellipsometric data with the B-spline model for the dielectric function. The larger the value of the smoothing parameter α, the smoother the result one can get. We will focus on application of the P-spline approach to dielectric function representation in spectroscopic ellipsometry data analysis.

The P-spline approach offers a number of advantages over well-established B-spline parameterization. First of all, it typically uses an equidistant knot arrangement which simplifies the construction of the roughness penalties and makes it computationally efficient. Since P-splines possess the “power of the penalty” property [4], the number and location of knots are no longer crucial, as long as there is a minimum knot number to capture all significant spatial variability of the data curves. We demonstrate the proposed approach by real-data case studies.

Keywords: Spectroscopic ellipsometry; Data analysis; Optical modeling; Dielectric function; Parameterization; Penalized splines; Optical metrology

References

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