Thin film thickness measurement error reduction by wavelength selection in spectrophotometry

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Abstract. Fast and accurate volumetric profilometry of thin film structures is an important problem in the electronic visual display industry. We propose to use spectrophotometry with a limited number of working wavelengths to achieve high-speed control and an approach to selecting the optimal working wavelengths to reduce the thickness measurement error. A simple expression for error estimation is presented and tested using a Monte Carlo simulation. The experimental setup is designed to confirm the stability of film thickness determination using a limited number of wavelengths.

1. Introduction
Thin film structures have many applications in industry. Current devices that contain multilayer thin film structures, such as liquid crystal and touch-screen displays and semiconductor devices, are mass-produced. Their quality often depends on the accuracy of the thin film parameters. The thickness is an essential property of a thin film that defines its physical characteristics. Therefore, a rapid yet precise technique for volumetric profilometry is needed to control the quality of film deposition during mass production.

A number of optical approaches are used to measure thin film thickness. Ellipsometry, spectrophotometry, and white-light interferometry are extensively applied for accurate and nondestructive film thickness measurement [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. All of these approaches allow us to measure not only the thickness of uniform thin films, but also the film thickness profile [1, 10, 5, 6, 7, 8]. Ellipsometry provides the most accurate thickness measurement, with errors as small as 5 Å [1]. Many measurements at different analyser positions are required to achieve this accuracy. In white-light scanning interferometry, the film thickness is computed by interferogram processing. Several intensity measurements at different optical path differences are needed to capture the required interferogram. Thus, spectrophotometry appears to be the most suitable approach for fast industrial profilometry.

Spectrophotometry is extensively applied for accurate and nondestructive film thickness measurement [3, 7, 5, 8, 4]. Several techniques have been developed for processing reflection spectra and determining the film thickness. A single-layer films thickness can be determined using a Fourier transform approach, but errors occur when the film thickness is less than 1 μm [13]. Nonlinear regression is a powerful approach that allows us to find the thickness of multilayer films or measure films that have unknown optical constants [3, 8]. The minimisation of the error function is usually a computationally intensive task, so nonlinear regression often
takes a considerable amount of time, although it can be accelerated by techniques such as direct phase calculation [6].

Quality monitoring systems must be able to measure the thickness of thin films with a lateral resolution of \((10^6 \text{ points/cm}^2)\). The speed of thickness determination becomes crucial in this task. One way to decrease the measurement and processing time is to reduce the amount of input information, but this also increases the thickness measurement errors.

When the number of wavelengths is limited, the measurement accuracy depends significantly on their values. The proper choice of wavelengths can considerably decrease the thickness determination errors.

Error analysis for multilayer film thickness determination by spectrophotometry is presented in [3]. The work in [14] presents an error analysis for a thickness determination technique based on the calculation of the optical parameters from three photometric quantities. The problem of choosing the wavelength values is not considered in the academic literature. In this paper, we introduce an approach to increasing the accuracy of thickness measurement by spectrophotometry using wavelength value selection. The optimal values are chosen using a priori information about the parameters of the film.

2. Theory
The reflection coefficient of a single-layer film can be expressed as follows:

\[
R = |r|^2 = \left| \frac{r_{12} + r_{23}e^{2i\beta}}{1 + r_{12}r_{23}e^{2i\beta}} \right|^2,
\]

where \(r_{12}\) and \(r_{23}\) are the Fresnel reflection coefficients for the airfilm and filmsubstrate interfaces, respectively; \(\beta = \frac{2i\pi}{\lambda} \hat{n}_2 d \cos(\theta_2)\); \(\hat{n}_2 = n_2 + ik_2\); \(d\) is the film thickness; \(\theta_2\) is the propagation angle of radiation in the thin film; \(n_2, k_2\) are refractive index and extinction coefficient of the film, respectively.

Nonlinear regression is a common technique for processing reflection spectra. Assuming that the reflectivity of a thin film is distributed normally with a variance \(\sigma_i^2\) for wavelength \(\lambda_i\), the film thickness is the value that minimises the residual sum of squares:

\[
\eta(d) = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \cdot \left[ R_t(\lambda_i, d) - R_m(\lambda_i) \right]^2,
\]

where \(R_t(\lambda_i, d)\) and \(R_m(\lambda_i)\) are the theoretical reflectance computed using (1) and the measured reflectance value, respectively.

3. Method to reduce thickness measurement error
The errors in film thickness determination by regression can be estimated using a linearised regression model. The standard deviation of the thickness can be expressed as [15]

\[
\sigma_d(d_0, \lambda_1, \ldots, \lambda_N) = \frac{1}{\sqrt{\sum_{i=1}^{N} \left( \frac{1}{\sigma_i} \frac{\partial R}{\partial d}_{d_0, \lambda_i} \right)^2}},
\]

where \(\frac{\partial R}{\partial d}_{d_0, \lambda_i}\) is the partial derivative value evaluated for thickness \(d_0\) and wavelength \(\lambda_i\).

The standard deviation depends on the derivative of the reflection, which depends on the thickness itself and the wavelength. Thus, the measurement error in a given thickness range can be decreased by selecting the optimal wavelengths.
For optimal wavelength selection, we introduce the objective function

$$Q(\lambda_1, \ldots, \lambda_N) = \min_{d \in [d_{\text{min}}, d_{\text{max}}]} \sum_{i=1}^{N} \left( \frac{1}{\sigma_i} \left| \frac{\partial R}{\partial d} \right|_{d=d_0, \lambda_i} \right)^2,$$

which is the minimum value of the expression under the square root in the denominator of (3). As the function $Q$ increases, the maximum thickness error in the given thickness range decreases. The values of $\lambda_i$ that maximise the function $Q$, are optimal.

Expression (3) was tested with Monte Carlo method [16]. For each thickness value, 2500 simulations were conducted. The reflectivity errors were sampled from the normal distribution $N(0, \sigma)$. The film thickness was computed by minimising function (2) using the Levenberg-Marquardt minimisation algorithm [17]. The standard deviation computed from the resulting values as a function of the thickness for $N = 3$ is illustrated in figure 1, where $N$ is the number of wavelengths. The simulation results show good agreement with the theoretical curve. The main standard deviation mismatch appears in the function extrema regions and is caused by nonlinearities in the function, which the employed model does not take into account.

To find the optimal wavelengths for measuring a MgF$_2$ film on BK7 glass substrate, function (4) was maximised using a differential evolution algorithm [18]. The thickness error for the obtained optimal wavelengths is shown in figure 1(b). The maximum standard deviation of the thickness error decreases from 5.24 $\mu$m for equally distributed wavelengths to 3.52 $\mu$m for the optimal wavelengths. The error value can be decreased by choosing a smaller thickness range.

The estimated error value for other numbers of wavelengths is shown in figure 2. The wavelength values were computed for each $N$ value and a thickness range of 30 – 1000 nm using the proposed approach. The shaded area of the plot characterises all the possible values of the standard deviation at the determined wavelengths.

The measurement error decreases considerably with increasing $N$ when the number of wavelengths is small (less than 10). Further increasing the number of wavelengths does not lead to such improvement.
Expression (3) can also be useful for estimating the error in multilayer film thickness measurement. The standard deviation of the $k$-th layer thickness can be found if the partial derivative is replaced by the corresponding $\frac{\partial R}{\partial d_k}$.

4. Experimental setup

Figure 3 shows schematic drawings of systems for film thickness measurement based on an acousto-optical tuneable filter (AOTF). A two-dimensional CCD sensor allows us to capture the spatial intensity distribution of light reflected from the sample, from which the spectral reflectances can be computed.

The setup shown in figure 3(b) has advantages over that in figure 3(a). The measurement error is proportional to the standard deviation of the noise [equation (3)], which can be improved by increasing the signal-to-noise ratio. The angle of light incidence can be adjusted to achieve the maximum image contrast and therefore the maximum signal-to-noise ratio. This angle equals the Brewster angle for a single-layer film deposited upon patterned structures.

![Figure 2. Standard deviation range for thickness measurement error as function of number of measured wavelengths. Wavelength values are optimised for thicknesses between 30 and 1000 nm.](image)

![Figure 3. Schematic drawings of spectrally tuneable profilometer.](image)
We also prefer the second setup because it does not contain a beam splitter, which causes considerable light intensity loss. The incidence angle can be tuned to achieve the best accuracy for single-layer and multilayer films deposited on substrates with various refractive indices.

To improve the spectral contrast, in our setup we used a double acousto-optical monochromator consisting of two non-collinear acousto-optical filters made of tellurium dioxide crystals and three polarisers (input, intermediate, and output) made of calcite crystals. The spectral contrast of a single AOTF is limited because of spectral side bands in its transmission function, which have the shape $\sin(x)/x$. These bands contain about 10%-20% of the energy, and using a double-AOTF design reduces that value to 0.3%-1%. In addition, using a double-AOTF design improves the image quality. The transmitted image quality is degraded by spectral drift of the image, the effect of different image scaling in two orthogonal directions, and nonlinear distortions. The use of a double-AOTF monochromator reportedly eliminates these effects because the second filter compensates for the image quality loss caused by the first AOTF [?].

The AOTF has the following characteristics:

- spectral range from 430 to 780 nm,
- 2 nm bandwidth,
- round input AOTF aperture with a diameter of 8 mm,
- 3° field of view,
- spatial resolution $800 \times 800$ elements.

Examples of spectral images are shown in figure 4. The thickness profile computed using the method described in section 2 is shown in figure 5. The experiment confirms that a unique solution can be found from three spectral reflectivity measurements.

5. Conclusion

Industrial systems for monitoring the quality of optoelectronic and semiconductor devices require techniques for thin film thickness measurement that are simultaneously fast and precise. We propose to use spectrophotometry-based systems with a limited number of wavelengths to
address this problem. It is necessary to limit the input information for these systems to provide sufficient processing speed, but this also increases the measurement errors. Methods of reducing the errors in this case are not considered in other works.

In this paper, we introduce an approach to minimising the measurement error for a known film thickness range by proper wavelength selection. The proposed technique will be useful for industrial quality monitoring applications where the target thicknesses is usually known, and it is expected to considerably increase the monitoring accuracy (up to 40% compared with that obtained using arbitrarily chosen wavelengths).

We designed an experimental setup based on AOTF to test the applied algorithms. The processing of captured images confirmed the stability of the obtained solutions.

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