Improving the measurement of thick and thin films with optical profiling techniques

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ABSTRACT

Optical profiling techniques, mainly confocal and white light interferometry, have demonstrated to be suitable techniques for characterization of transparent thick films. Measurements are carried out by vertically scanning the upper and lower film interfaces. Thickness of the layer is determined from the two peaks in the confocal axial response or from the two sets of interference fringes developed during the vertical scan. The 3D topographies of the upper and lower interfaces of the film can also be obtained. Measurements of photoresists or oxide coatings are typical examples of thick film characterization. On the other hand, measurement of thin films is considered to be a very difficult application to carry out with most optical imaging profilers. A film should be considered as thin when the two peaks obtained along the vertical scan become unresolved. We introduce new methods based on confocal techniques, which make it possible to measure sub-micrometric layers on structured samples. These techniques are based on the comparison between the axial responses obtained in areas where the film is present and those in other areas where only the substrate is present. This method has been successfully used for thickness assessment of several samples, such as a set of calibrated Si-SiO_2 layers.

Keywords: Optical profiler, shape measurement, thickness measurement, thick film, thin film, confocal profiler.

1. INTRODUCTION

One of the applications considered most difficult to carry out with most optical imaging profilers, is the characterization of stratified media obtained from the superposition of micro or sub-micrometric layers of dissimilar materials. These media are used nowadays in many fields, such as semiconductors, flat panel displays, optical coatings and data storage. Research activities and industry quality control applications require the accurate characterization of a range of properties of stratified media, including film thickness, refractive index and 3D surface shape of the upper and lower interfaces of the film. Because of the refractive-index variations in the axial direction, visible light is reflected in the various interfaces. As a result, some reflected wavefronts are superposed giving rise to interference patterns, which are difficult to understand in terms of surface topography and layer thickness. This may cause conventional optical profiling techniques to obtain strange results[1,2].

It is common to distinguish between thick and thin films. A film is considered to be thick when it is possible to discriminate the two peaks developed during the vertical scan. On the contrary a film should be considered as thin when the two peaks become unresolved. Note that a film may behave as thick when it is measured with a confocal profiler with a high NA objective and may behave as thin if it is observed with a low NA objective. In the same way a film may behave as thick if it is measured with a white light interferometer and may behave as thin if a narrow band light source with larger coherence length is used. Therefore the limit between thick and thin behavior of a film being measured using optical techniques does not only depend of the film itself. From the practical point of view this limit

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can be considered very close to 1 μm for a white light interferometer and very close to 1.5 μm when a confocal profiler is used.

In this paper we will focus our attention on the understanding and the improvement of the characterization of thick and thin films with confocal profilers. Interferometers are also very interesting tools for thickness measurement applications, but theoretical approach is slightly different and they will be treated in a future contribution.

2. RIGOROUS THEORETICAL MODEL

According to the scalar, non-paraxial Debye theory of axial imaging[3], in a confocal microscope the sample is illuminated by an angular spectrum of plane waves[2-7]. The illumination pinhole acts as an infinitely small secondary light source and therefore the effective illumination is coherent. Each component of the spectrum of plane waves is reflected on the surface of the sample. The effect of the confocal aperture is to integrate over the amplitudes of the reflected angular spectrum. Therefore the detector is considered to be infinitely small and incoherent.

When the sample is scanned along the *z* axis in the neighborhood of the focal point, and assuming that sine condition holds, the detected axial response will be given by:

$$I(x,y,z) = \int_{\lambda_0-\Delta\lambda/2}^{\lambda_0+\Delta\lambda/2} \phi(\lambda) \left| \int_0^{\theta_0} R(x,y,\theta) P^2(\theta) \exp(2ikn_0 z\cos\theta) \sin\theta\cos\theta \, d\theta \right|^2 d\lambda \qquad (1)$$

where k is the wave number ($2\pi/\lambda$), n_0 is the refractive index of the medium surrounding the surface of the sample and θ is the angle of convergence, which is limited by the numerical aperture of the microscope objective ($n_0 \cdot \sin\theta_0 = NA$). $R(x,y,\theta)$ is the reflection coefficient for linearly polarized illumination, which depends on the film and substrate features at each point (x,y) within the field of view and $P(\theta)$ is the pupil function. Since the same microscope objective is used for illumination and detection the pupil function needs to be considered twice in expression 1.

If we consider a transparent dielectric film of refractive index n_l on a dielectric substrate of refractive index n_s, $R(x,y,\theta)$ is the appropriate Fresnel reflection coefficient, which can be found in many references[4,8,9] and takes into account effects such as multiple reflections, interferences between wavefronts reflected on the interfaces and beam depletion. If the film and/or the substrate are conductive media, then Fresnel reflection coefficient has to be expressed as a function of the corresponding complex refractive indexes of the layer $\tilde{N}_l$ and the substrate $\tilde{N}_s$[10] .

Most of the references related to axial imaging theory use monochromatic illumination and pupil function $P(\theta)=1$, which means uniform illumination at the aperture stop and an aberration-free optics. Instead, as our aim is to reproduce the axial responses obtained with different NA objectives in many different thick and thin films made of dispersive materials, even when light sources with very short wavelengths within the visible spectrum are used, our model will also take into account the following features:

(a) A light source with normalized spectral radiant flux $\Phi(\lambda)$ with peak emission at λ_0 and spectral bandwidth $\Delta\lambda$.
(b) Dependence of the refractive indexes of the film and the substrate with the wavelength $\tilde{N}_l(\lambda)$ and $\tilde{N}_s(\lambda)$.
(c) Non-uniform illumination at the aperture stops, particularly for low NA objectives.
(d) Phase deviations on the pupil function to include spherical aberration, particularly for high NA objectives.
(e) Phase deviations on the pupil function to include longitudinal chromatic aberration, particularly for low NA objectives and short wavelength illumination.

All parameters involved in the model have been carefully assessed[7]. Some of them are reported in the following sections, in which the axial responses obtained with the rigorous theoretical model are compared with experimental results obtained with an optical imaging profiler in different surfaces containing thick and thin films.

3. THICK FILM MEASUREMENTS

A film is considered to be thick when the axial response shows two well resolved peaks at the two parallel reflecting interfaces. The widths of the peaks are reduced when the NA of the objective increases and the distance between the peaks increases with the thickness of the film.

Figure 1 shows the experimental axial responses of a 144.1-μm-thick glass sheet (n_l=1.52) obtained with different objectives. It also shows a bright-field image of the edge of the glass sheet obtained with a 50X EPI objective, which was used to asses the real thickness of the sample. All these measurements were carried out with an optical imaging profiler PLμ 2300 from Sensofar-Tech.

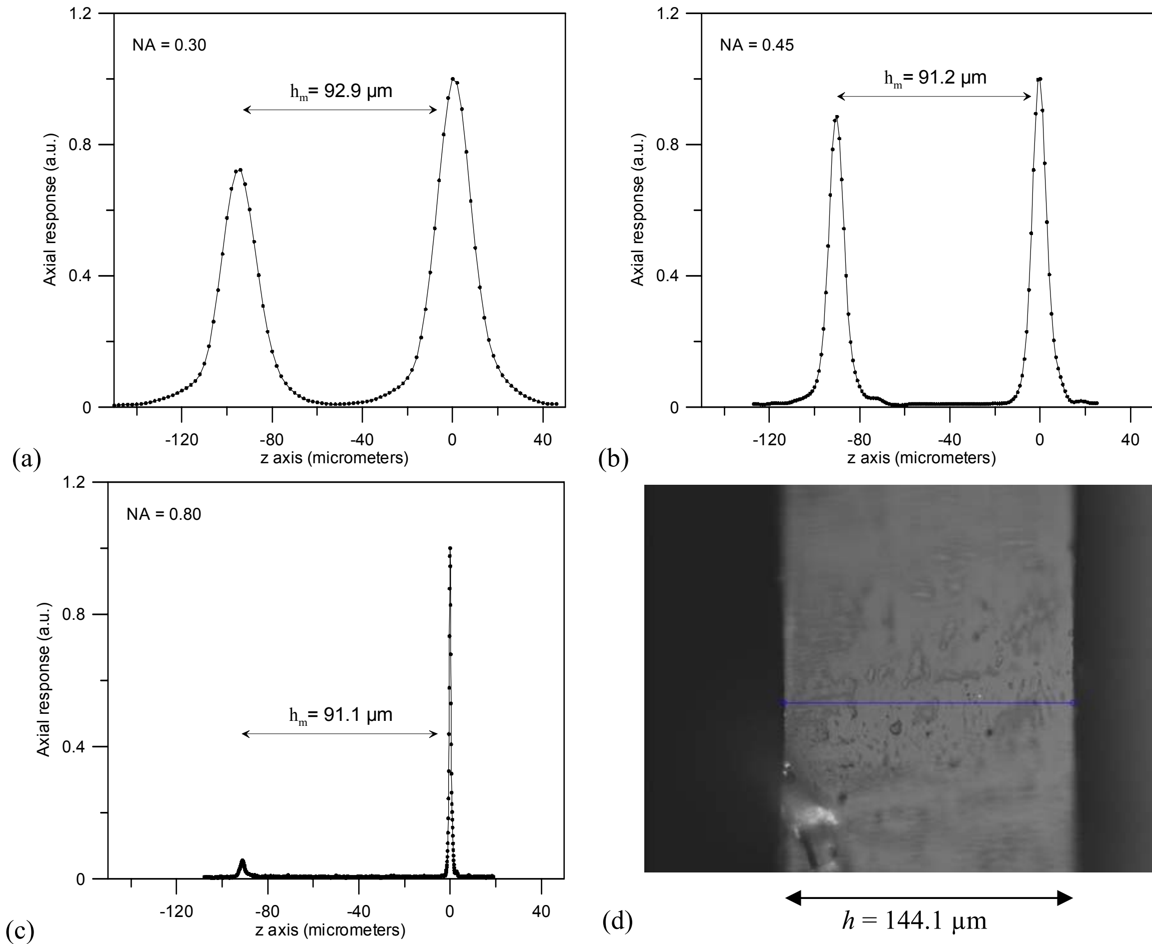


Figure 1. Axial responses obtained in a confocal profiler when a glass sheet is scanned through the confocal depth of focus. (a) objective 10X, NA=0.30 (b) objective 20X, NA=0.45 (c) objective 50X, NA=0.80 (d) bright-field image of a section of the glass sheet, objective 50X.

The measured separation of the peaks h_m is very different from the real thickness h of the sheet. Figure 2 shows the experimental results of the correction factor h_m/h obtained from the axial responses measured with different NA. Results predicted by the rigorous theoretical model introduced in Section 2 are also plotted. The agreement is extremely good for all NA.

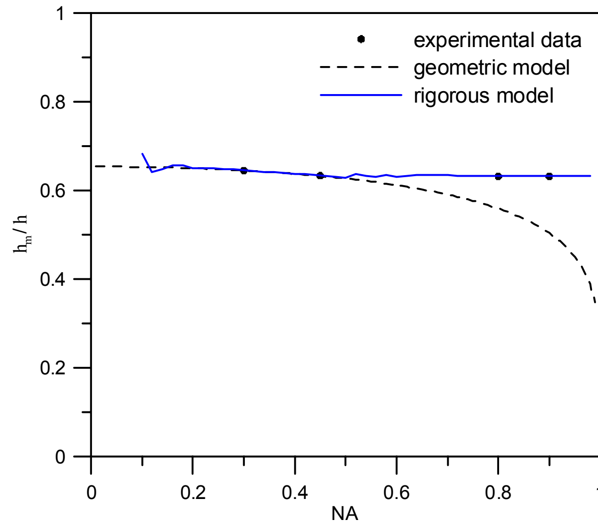


Figure 2. Experimental values h_m/h obtained from the axial responses measured with different NA for a 144.1-µm-thick glass sheet. Results predicted by the rigorous theoretical model are plotted in continuous line and results predicted by the simple geometrical model are also plotted in dashed line.

The relationship between h_m and h can be also predicted using a much simpler geometrical model[11].

$$\frac{h_m}{h} = \frac{\int_0^{\theta_0} \sin\theta d\theta}{\int_0^{\theta_0} \frac{\left(n_l^2 - \sin^2\theta\right)^{1/2}}{\cos\theta} \sin\theta d\theta} \tag{2}$$

This model just takes into account two factors: (i) depth distortion due to the index of refraction n_l of the medium and (ii) the spherical aberration caused by focusing through a refractive medium.

Results for the correction factor h_m/h predicted by the geometrical model are also plotted in Fig. 2. The agreement is fairly good for the lower NA objectives but is less satisfactory for NA values above 0.5. While this method is not strictly correct, it offers a quick method for calculating the correction factor that can be used for objectives with a low NA.

Some more thickness measurements have been conducted with the optical profiler in confocal mode, even in thinner samples in which the two peaks are very close to become unresolved[12]. In all of them a very good agreement between the experimental results and the rigorous theoretical model has been demonstrated.

4. THIN FILM MEASUREMENTS

A film is considered to be thin when the two peaks of the axial response become unresolved. Below this limit effects such as multiple reflections and interferences between wavefronts reflected on the interfaces become very significant so that optical profilers were considered to be unsuitable to measure thickness and provide correct 3D shapes[4].

To overcome this limit we introduce a new method, which makes it possible to measure thin films on structured samples. The new method is outlined in Fig. 3 and it is based on the comparison between the axial responses obtained in the same z-scan in areas where the film is present and those in other areas where only the substrate is present.

In a thick film the measured thickness h_m was the z-distance between the two resolved peaks in the axial response obtained at a given position *(x,y)* of the surface after scanning the sample along the z-axis (Fig. 3a). With the new approach, the measured thickness h_m is the z-distance between the peak obtained in a position (x_s, y_s) where there is only substrate, and the larger peak obtained in a position (x_l, y_l) where there is a thin film of thickness *h* over the substrate (Fig. 3b).

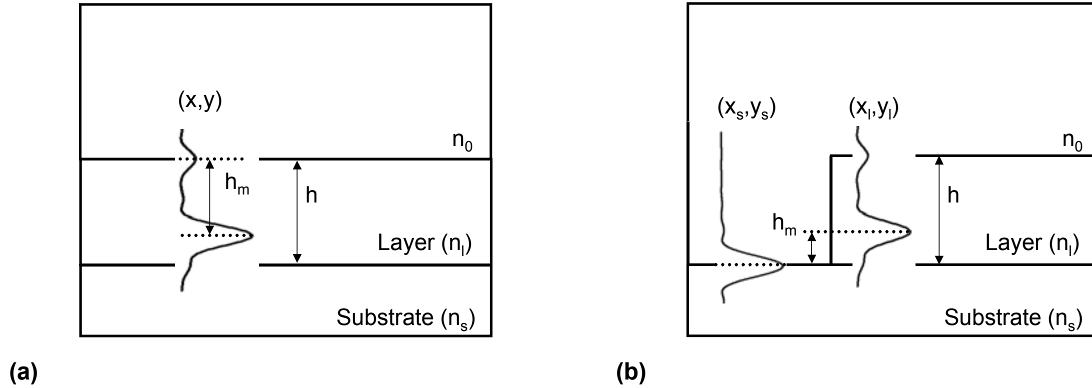


Figure 3. Measured thickness h_m obtained in a thick film (a) and in a thin film with the new approach (b)

Therefore, the new measured thickness is obtained as:

$$h_m = z_{peak}(x_l, y_l) - z_{peak}(x_s, y_s), \tag{3}$$

where the peaks (z_{peak}) are obtained from the axial responses. It is important to point out that confocal profilers assign the z-coordinate corresponding to the maximum of the axial response measured along the z-scan to each point *(x,y)*. Therefore, the new definition of h_m is exactly the step height measurement obtained when a topography or a profile are measured on a structured sample using the confocal technique[13-15]. This is highly advantageous as it enables the use of any confocal profiler to perform these measurements.

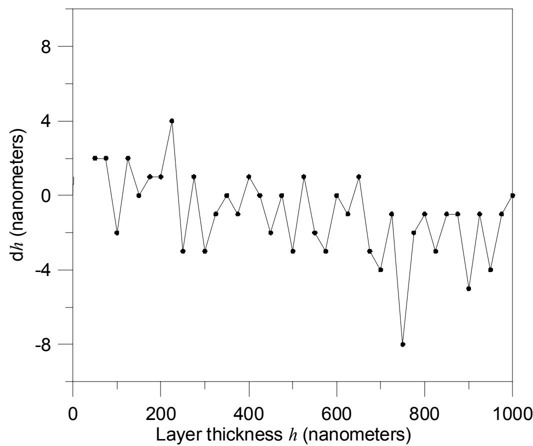


Figure 4. Deviations from the nominal thickness as a function of layer thickness.

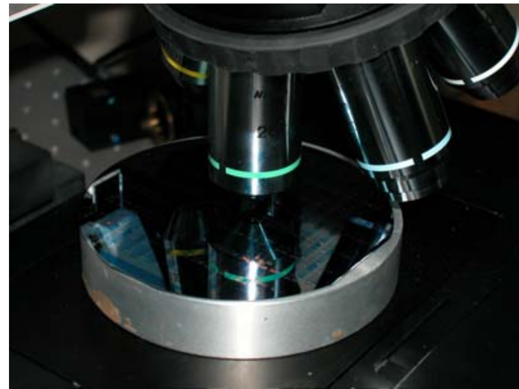


Figure 5. One wafer belonging to the set of samples of a layer of SiO_2 on a Si substrate.

To check the new method a set of wafers was prepared at the *Centro Nacional de Microelectrónica (CNM-CSIC)*. On each wafer, layers of SiO_2 were grown or deposited on Si substrate. After growth or deposition the layers were patterned by a standard photolithographic process. Nominal thicknesses range from 1000 nm (wafer 1) to 50 nm (wafer 39) with a 25 nm interval. The real thickness of the SiO_2 layer of each sample was measured using a contact profiler. Figure 4 shows the deviations from the nominal thickness as a function of layer thickness; these deviations are below 8 nm.

To check the ability of the rigorous theoretical model to reproduce the confocal axial response I(z) and the relationship between the measured thickness h_m and the real thickness h we carried out several measurements on the set of samples with the same optical imaging profiler PLμ 2300 from Sensofar-Tech. One of the wafers is shown in Figure 5 while being measured in the confocal mode. Table 1 summarizes the magnifications and NA's of the microscope objectives CFI60 LU Plan EPI from Nikon that were used in the confocal mode, as well as the repeatability values corresponding to the z-coordinates of the measured surface.

Objective CFI60 LU plan EPI	10X EPI	20X EPI	50X EPI	100X EPI	150X EPI
Numerical Aperture	0.30	0.45	0.80	0.90	0.95
z-repeatability σ (nm)	50	20	4	3	2

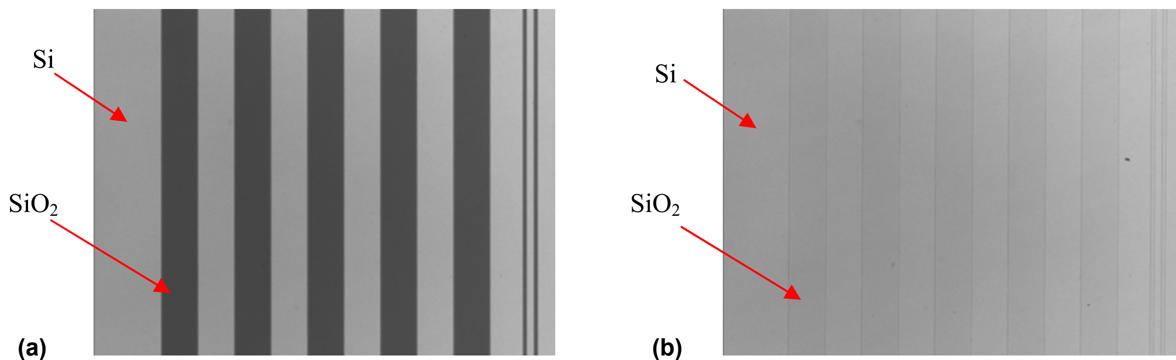
Table 1. Objective specifications

The first set of measurements consists of acquiring experimental axial responses I(z) and comparing them to calculated ones. Instead of acquiring a topography for each wafer, two axial responses are acquired, one at a position where there is just the Si substrate and the other at a position where there the SiO_2 layer is.

Figures 6a and 6b show bright field images corresponding to wafer 31 (h=250 nm) and wafer 35 (h=150 nm) obtained using objective 10X EPI. There is an indication of wafer layout (Si and SiO_2 areas) superimposed on the images.

Figure 6c shows the intensity axial responses obtained on wafer 31. At first sight the Si and SiO_2 axial responses only differ in intensity I(z). However, the peak positions are not the same. The difference between peak positions is small (≈1.5 μm) in comparison to FWHM (≈ 20 μm).

Figure 6d shows the intensity of the axial response peak as a function of layer thickness. While the intensity of the axial response peak corresponding to Si presents small variations, the intensity of the axial response peak corresponding to SiO_2 varies periodically. The variations in peak intensity are due to the interference between the wavefront reflected at the *air–*SiO_2 interface and the wavefront reflected at the SiO_2*–Si* interface.



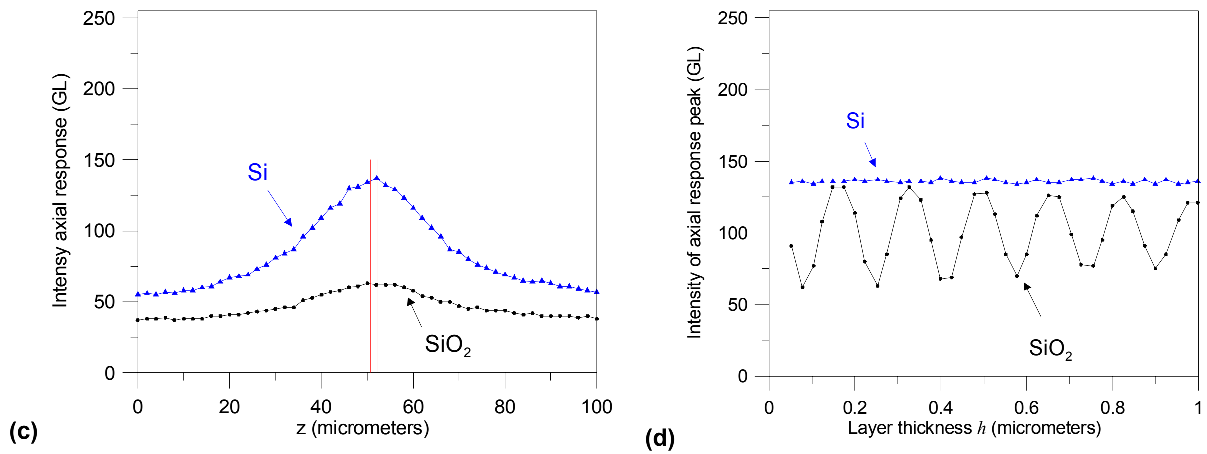


Figure 6. Test for acquisition of axial responses at Si and SiO_2 positions using objective 10X EPI (NA 0.30). Light source is a blue LED. (a) Bright field image of wafer 31 (*h*=250 nm) (b) Bright field image of wafer 35 (*h*=150 nm) (c) Si and SiO_2 axial response of wafer 31 (d) Si and SiO_2 peak intensity as a function of layer thickness *h*.

Variations in peak intensity as a function of layer thickness can be used to evaluate the agreement of the axial responses calculated using the model with the experimental data. For purposes of this comparison, the peak intensities are standardized so that peak intensity corresponding to Si positions is set to unity. Figure 7 shows the experimental and model standardized SiO_2 peak intensities for objectives 10X, and 50X EPI.

Agreement between the experimental and calculated data is fairly good for all objectives. From these results it can be concluded that the model is able to correctly reproduce the interference phenomenon introduced by the presence of the layer regardless of the NA value.

The second set of measurements consists of acquiring a 3D topography for each wafer. Figure 8 shows a typical display of profile and topography obtained with this system in the confocal mode.

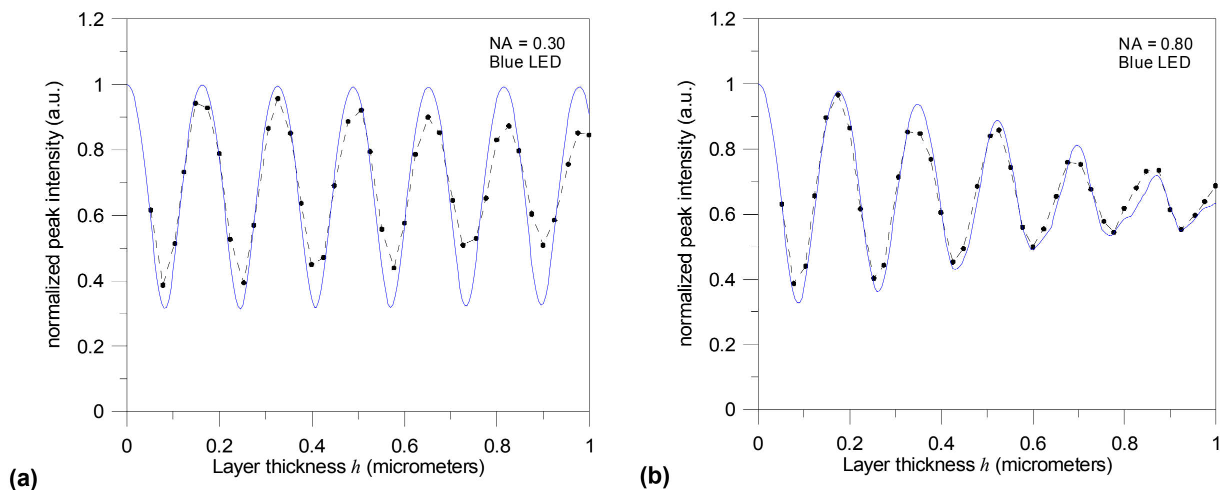
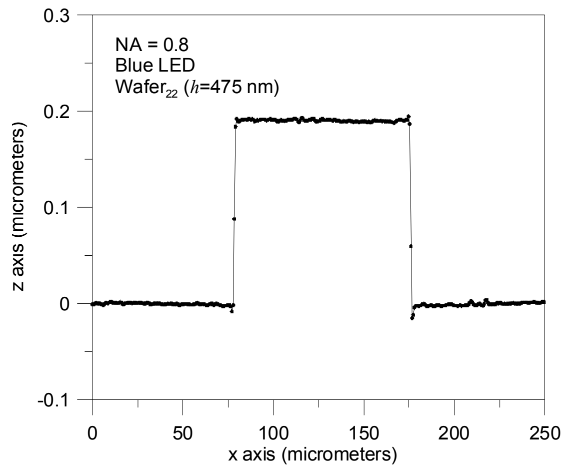


Figure 7. Standardized peak intensity measured with the different objectives (dots and dashed line). The peak intensity obtained from the theoretical approach is also shown (continuous line). Light source was a blue LED.
(a) 10X EPI; NA 0.30 (b) 50X EPI; NA 0.80.



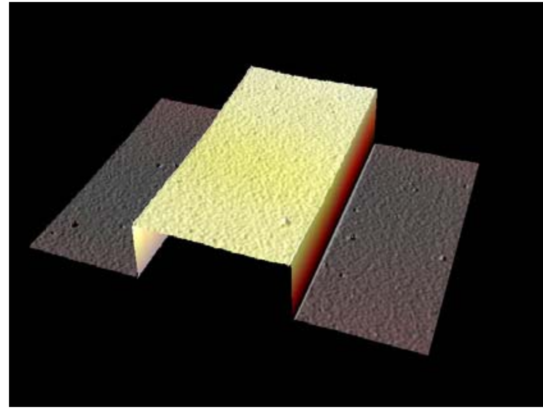
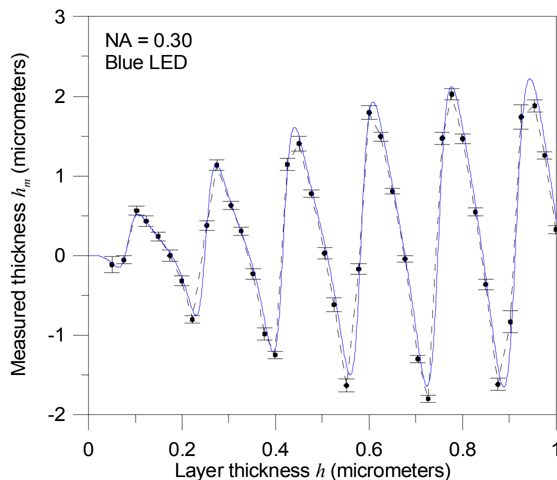


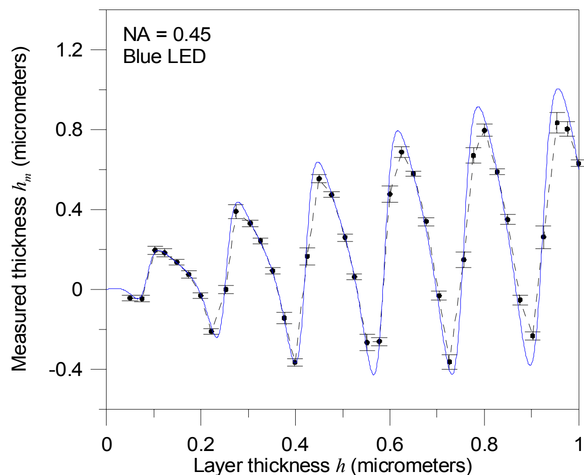
Figure 8. Profile and topography displays obtained with the confocal mode. The objective used is the 50X EPI (NA=0.80) and light source is a blue LED (λ=472 nm). Wafer 22 (*h*=475 nm); h_m =190 nm.

The thicknesses of the layers h_m were measured in some selected positions of the layout for the different samples according to the following procedure:

(i) The samples were positioned in the profiler, focused and scanned along the z-axis. As a result, the 3D topographies of the surfaces were obtained at the different selected positions of the layout.
(ii) The topography was leveled (by subtracting a plane term) to remove the small misalignments (tip and tilt) of the surface of the sample in relation to the optical axis of the profiler.
(iii) The histogram of the leveled topography was displayed. The thickness of the layer h_m was measured as the separation of the two peaks in the histogram. In addition, a measurement of the dispersion of the values was also obtained from the histogram as the full width at half the maximum of the histogram peak corresponding to the SiO_2 layer.

Note that the PLμ 2300, as most optical profilers, assigns to each point (x,y) of the surface the z-coordinate corresponding to the maximum of the axial response measured along the z-scanning. Thus, the thickness of the layer measured according to the procedure described above will be exactly the same as the one defined on the theoretical approach.





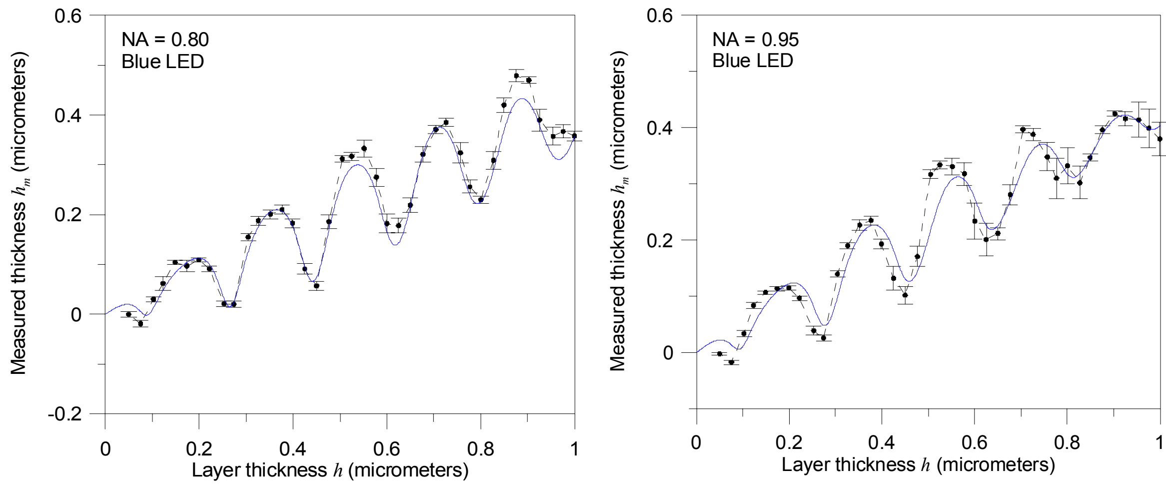


Figure 9. Thicknesses of the SiO_2 films measured with the different objectives in the set of samples (dots). The measured thickness h_m obtained from the theoretical approach is also shown (continuous line). Light wavelength is 472 nm.

The thicknesses of the SiO_2 layers measured with the different objectives in the set of samples have been plotted in Fig. 9. The relationship of the measured thickness h_m and the real thickness h obtained from the theoretical approach is also plotted in continuous line. It can be concluded that agreement between theoretical and experimental data is fairly good.

Demonstrated agreement between theoretical model and experimental results makes it possible to introduce a new indirect method for measuring the real shape of structured samples containing thin films and substrates of dissimilar materials. The method is based on the comparison between the axial responses obtained in areas where the film is present and those in other areas where only the substrate is present. As we claimed in a previous work containing preliminary results[2], this method enables confocal profilers to measure the thickness of layers on the sub-micrometric scale for the first time.

Figure 10 shows a block diagram of the indirect method. First, topographies of the sample are measured using at least two different NA's. For each NA a value of measured film thickness h_m is obtained as the average height difference between areas where there is only substrate and areas containing the film being measured. The set of film thickness values h_m (NA) is the measured data.

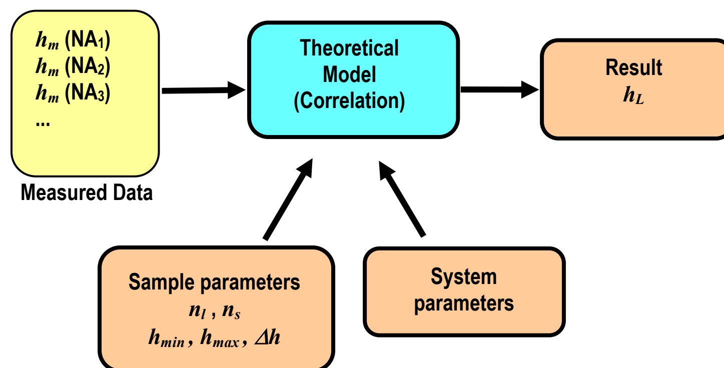


Figure 10. Diagram of the method for thickness measurement of structured surfaces containing dissimilar materials

Second step of the method consists of calculating the values of measured film thickness $h_{m,model}$ using the rigorous theoretical model. Several parameters must be defined to determine the overall accuracy of the calculations. Sample parameters, which define sample structure, include the refractive index of sample materials ($\tilde{N}_l$, $\tilde{N}_s$) and minimum and maximum film thickness, h_{min} and h_{max}. The limits of thickness range must be selected to ensure that it contains real thickness h. Thickness step Δh must also be defined and is used to obtain a set of thicknesses h_i varying from h_{min} to h_{max}. The system parameters, which define the confocal system used to perform the measurements, include, at least, light source central wavelength λ_0 and NA of the different microscope objectives. Whenever it is considered necessary, characterization of aberrations and spectral bandwidth of the light source should be also provided.

The third step consists of calculating for each NA the difference between the experimental measured thickness h_m and the theoretical measured thickness $h_{m,model}$ as a function of film thickness h. Real film thickness will give rise to differences very close to zero for all NA. An error function is defined as the inverse of the of the sum of the square of the differences between theoretical measured thickness $h_{m,model}$ and experimental measured thickness h_m:

$$Error\ function\left(h_i\right) = \frac{1}{\sum_{NA}\left[h_{m,\mathrm{mod}\,el}\left(h_i, NA\right) - h_m\left(NA\right)\right]^2} \tag{4}$$

The error function's maximum is obtained at film thickness $h_i = h_L$, which is assumed to be the best estimate for real film thickness with a sampling error of Δh.

As an example to illustrate the description of the method we can use wafer 10. Nominal thickness of the SiO_2 film is 775 nm whereas the real thickness is $h = 776.6$ nm. 3D topographies were acquired with different NA's using the PLμ 2300 optical profiler in confocal mode. Measured data h_m are listed in table 2.

Objective CFI60 LU plan EPI	10X EPI	20X EPI	50X EPI	100X EPI	150X EPI
Numerical Aperture	0.30	0.45	0.80	0.90	0.95
h_m	2025 nm	670 nm	256 nm	297 nm	310 nm

Table 2. Measured data obtained on wafer 10 (h = 776.6 nm) using the PLμ 2300 optical profiler in confocal mode

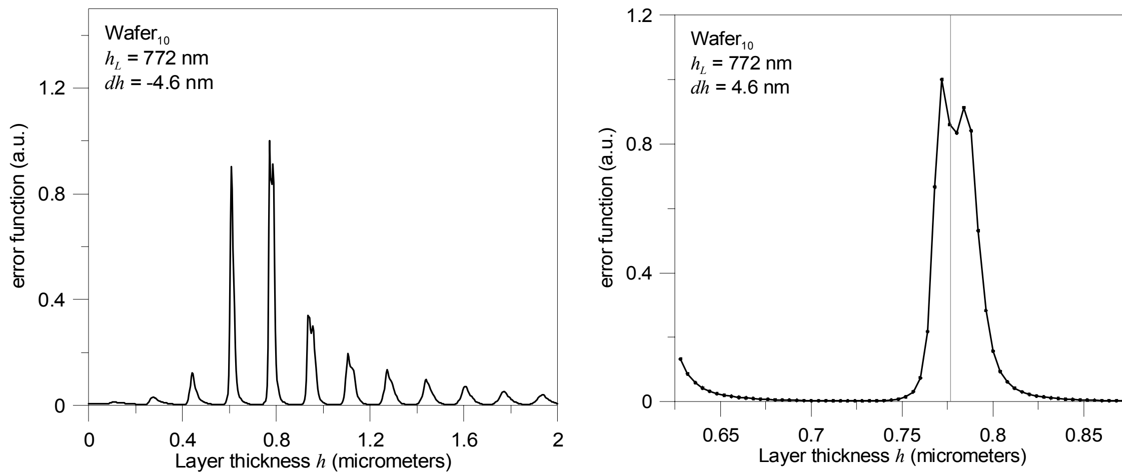


Figure 11. Error function for wafer 10. The maximum determines layer thickness: h_L = 772 nm. Vertical line marks real thickness (h = 776.6 nm). Measurement error is 4.6 nm

The refractive indexes of SiO_2 and Si, at blue wavelength, were set to 1.46 and 4.44, respectively. Figure 11 shows the result of the error function for two ranges of film thicknesses, a coarse one from 0 to 2 μm and a finer one from 625 to 875 nm. Layer thickness step Δh was set to 2 nm. The maximum of the error function is obtained at h_L = 772 nm, which means that measurement error of film thickness is 4.6 nm. The accuracy of the parameters used to generate $h_{m,model}$ determines the overall accuracy of the method. On the other hand, film thickness step Δh determines the resolution. Resolution could be easily improved using smaller values for film thickness step Δh, but this would raise a lot the calculation time.

Figure 12a shows the results for the complete series of wafers when a fine range centered on the nominal film thickness of each wafer is used. Figure 12b shows the differences between measured film thickness h_L and real film thickness h. It is worth noting that results are very good for all wafers. The maximum error is 22.1 nm, the mean error is 2.8 nm and the standard deviation of errors is 4.5 nm.

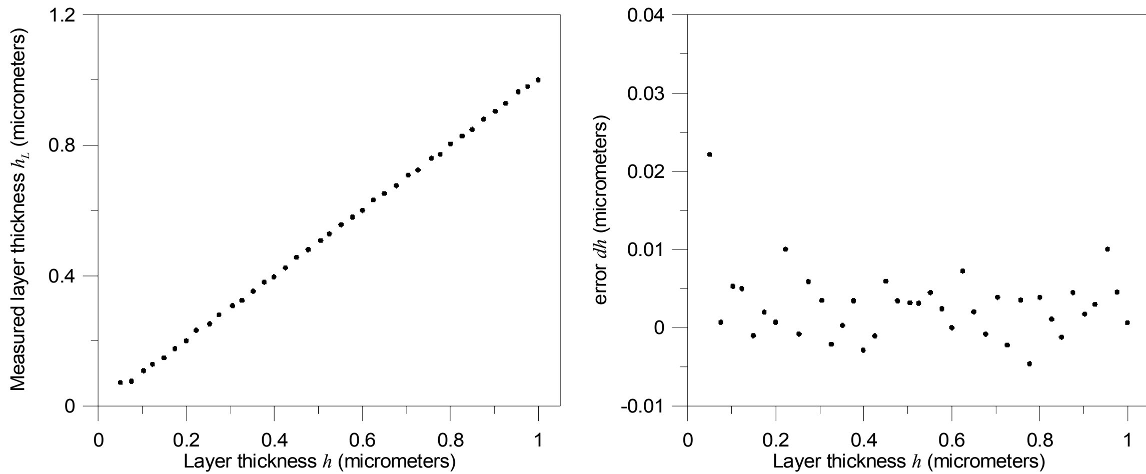


Figure 12. Thickness measurement results for the complete series of wafers.
(a) h_L as a function of layer thickness h, (b) measurement error $dh = (h_L - h)$ as a function of layer thickness h.
Mean measurement error is 2.8 nm and standard deviation is 4.5 nm.

To check the applicability of the new technique for sub-micrometric thickness measurements, three samples different than the series of wafers were measured. Table 3 lists the sample name, refractive index of the layer and the substrate at blue wavelength, nominal thickness and measured thickness h_L obtained with the new technique.

Sample	n_l	n_s	h	h_L	*Error*
Indiumtinoxide (ITO) on glass	2.07	1.5	133.9 nm *	127 nm	6.9 nm
Polyvinylalcohol on Si	1.5	4.44	69.4 nm *	69 nm	0.4 nm
Alq3 on Si	1.80	4.44	60 nm **	65 nm	5 nm

Table 3. Sample name, refractive index of the layer and the substrate at blue wavelength,
film thickness h and film thickness h_L obtained with the new technique
(*) film thickness measured with an Alpha Step IQ contact system (**) nominal thickness

On the basis of the results presented in this section it can be concluded that the new technique is very good and able to provide thickness measurements of thin films with an error of accuracy in the order of ±5 nm.

5. CONCLUSIONS

A rigorous theoretical model based on the previous work of C.J.R. Sheppard has been developed for simulating the axial response obtained with a confocal profiler in the presence of a film. The model has been modified to take into account light bandwidth, dispersive materials, non-uniform illumination and system aberrations.

Experimental results obtained in samples containing thick films have shown good agreement with the theoretical simulations, even with high NA objectives. Thin film behavior is found where the two peaks in the axial resolution become unresolved. Below this limit confocal profilers seem to be unsuitable for film characterization.

To overcome this limit a new method has been introduced. The method is based on the comparison of the axial responses obtained in areas of the surface where there is a film and in other areas where there is just the substrate. Experimental results obtained in a calibrated set of wafers containing SiO_2 thin films deposited on Si substrate have shown good agreement with the theoretical simulations. To our knowledge, this approach enables optical profilers to measure the thickness of films on the sub-micrometric scale for the first time.

6. ACKNOWLEDGMENTS

This research was supported by the Ministerio de Ciencia y Tecnología, Spain. The project (Ref. DPI2002-01018) was partially financed by the EU-FEDER program. The authors would like to thank the *Centro Nacional de Microelectrónica (CNM-CSIC)* for supplying the structured samples used to obtain the experimental results.

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