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Ellipsometric inline inspection of dielectric substrates with nonplanar surfaces

Ellipsometrische Inline-Inspektion dielektrischer Substrate mit nonplanaren Oberflächen

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Abstract: An analytical solution for the determination of either angle of incidence (AOI) and the refractive index from combined ellipsometric and reflectometric measurements at dielectric substrates is presented. The solution is of special importance for retroreflex ellipsometry (but not limited to this application). Overcoming the geometric restrictions of conventional ellipsometers, the patented retroreflex ellipsometry can detect changes of intensity and the state of polarization in or at test objects even with curved surfaces. In contrast to conventional ellipsometers where the AOI is set by the adjustment procedure, the AOI is usually unknown in retroreflex ellipsometry. For quantitative analysis, the knowledge of the AOI is nevertheless essential. The proposed combination of retroreflex-reflectometry and retroreflex-ellipsometry opens the path to precise measurements of either surface geometry and index of refraction of nonplanar dielectric substrates (e. g. surfaces of freeform optics).

Keywords: Retroreflex ellipsometry, ellipso/reflectometry, curved surface, nonplanar, glass, dielectric.

Zusammenfassung: Analytische Formeln zur gleichzeitigen Bestimmung des Einfallswinkels und des Brechungsindex dielektrischer Substrate aus reflektometrischen und ellipsometrischen Messwerten werden vorgestellt. Diese Lösungen sind von besonderer Bedeutung für die Retroreflex-Ellipsometrie (aber nicht auf diese beschränkt). Die patentierte Retroreflex-Ellipsometrie überwindet die geometrischen Restriktionen konventioneller Ellipsometer und erlaubt dadurch die Detektion von Änderungen der Intensität und des Polarisationszustands selbst an Proben mit gekrümmten Oberflächen. Bei konventionellen Ellipsometern wird der Einfallswinkel eingestellt und ist somit genau bekannt. Im Gegensatz dazu ist er bei der Retroreflex-Ellipsometrie per se unbekannt. Eine quantitative Auswertung ellipsometrischer Daten ist jedoch nur bei Kenntnis des Einfallswinkels möglich. Die vorgeschlagene Kombination von Retroreflex-Reflektometrie und Retroreflex-Ellipsometrie eröffnet somit die Möglichkeit zur gleichzeitigen präzisen Bestimmung der Oberflächengeometrie und des Brechungsindexes nonplanarer dielektrischer Substrate (z. B. Oberflächen von Freiformoptiken).

Schlagwörter: Retroreflex-Ellipsometrie, Ellipso/Reflektometrie, gekrümmte Oberflächen, nonplanar, Glas, dielektrisch.

1 Introduction

Objects with tightly controlled physical properties (e. g., glasses, functional films) are becoming more and more important in industrial production processes because product reliability is the most important factor in mass production. They are to be found not only throughout the area of photonics and semiconductor but also in a growing number of other sectors, e. g., the automobile industry, metal coatings and glass production. Industry requires sensitive measurement systems to improve production (e. g., control and efficient use of resources), and provide quality assurance. These systems must offer 100 percent inspection of the physical properties of the manufactured objects and/or surfaces (measurement processes with material detection).

Ellipsometry is a widely used optical method for the characterization of materials and thin films [4]. It provides high precision, sensitive and non-destructive measurements which can be used for process monitoring of surfaces and transparent objects. With this technique, the surface of the test object is illuminated with polarized light. Dependent on the object's optical properties, the intensity and the state of polarization change as the light is reflected

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at or transmitted through the sample. The changes are described by Fresnel's equations [2]. The intensity and the polarization state of the reflected or the transmitted light are measured using a detector. In ellipsometry, it is usual to calculate the parameters R resp. T, Ψ and Δ to describe the changes in intensity and polarization at the object. These parameters and the two angles of inclination of the sample surface are the input values for the object model. The object model describes the basic physical structure of the test object (substrate, number and types of films etc.) as well as previous knowledge relating to the inspection task. The model uses these known and measured parameters to determine the unknown physical properties of the observed object element. The relevant parameters for the object model are the refractive index, the extinction coefficient, birefringence, dichroism, depolarization, and the path through the material, if applicable. If several materials are involved (e. g., multi-layer films), the parameters for all the materials involved are included in the model. In principle, these parameters and the values derived from them (e. g., tensions and tensile forces) can all be measured using ellipsometry.

Ellipsometry is already established as a standard laboratory tool in many areas, e. g., special applications in biology and medicine [19], and the measurement of ultrathin films ranging in thickness from a fraction of an atom (incomplete films) to several micrometers with outstanding accuracy [10]. It also has applications in some areas of the characterization of materials, such as the detection of contaminants [15], determination of the degree of crystallinity [16] or monitoring corrosion of alloys [11]. Despite the many possibilities offered by the technique, it is very rarely used in industrial applications or only in exceptional cases because of the geometrical limitations of conventional ellipsometry. Measurements with conventional ellipsometers are only possible for plane surfaces or plane surface elements (with respect to the measurement beam). Even slight misalignments from the ideal reflection or transmission setting might lead to significant experimental errors. For larger misalignments, it is mostly even not possible to get any evaluable signals.

In order to overcome the limitation of ellipsometry, retroreflex ellipsometry was developed at Fraunhofer IOSB [7, 8]. In this configuration, a retroreflector is used to reflect the light from the sample back to the detector on the same beam path. The polarization effect of the retroreflector is the same as that of an ideal mirror. The acceptable angle deviation of the surface is up to 30°. For precise ellipsometric measurements of dielectric substrates, a new method is proposed to calculate optical properties and angles of incidence for isotropic dielectric materials by combining reflectometric and ellipsometric measurement.

2 Related work

Alternative concepts of ellipsometric measurements at non-planar surfaces are found in the literature. Haberland et al. [6] compensated the substrate wobbling by placing the sample at the center of a spherical mirror to reflect the beam back to the detector. Neuschaefer-Rube and Holzapfel [14] used an off-axis focusing optics to measure surface geometry and material distribution simultaneously. Lee et al. [12] measured the azimuth deviation of the polarizer to estimate the curvature and the refractive index of a plano-convex lens. Ghosh et al. [5] analyzed the Stokes reflectance field of circularly polarized spherical illumination to estimate the refractive index and the shape of specular dielectric materials. Tsuru [18] used circularly polarized light to illuminate the object for three-dimensional shape measurement. Li et al. [13] established a Mueller matrix model of curved samples to measure the film thickness of a spherical lens. Nevertheless, there are some drawbacks or limitation in these methods for general industrial applications. The methods from Haberland et al., Neuschaefer-Rube and Holzapfel, and Lee et al. are only suitable for samples with small angle variation. The method from Ghosh et al. needs complicated light sources to generate different incident lighting directions. The model from Tsuru is based on a known refractive index of the sample and special illumination environment. There, prior measurement of the sample is necessary. The method from Li et al. fitted the Mueller matrix spectrum to estimate the radius of the sample and the thickness of the film, but this fitting procedure and the adjustment of the detector are time-consuming and not suitable for inline measurement systems.

3 Retroreflex ellipsometry

3.1 Restriction of conventional ellipsometry in inline measurement

The following factors must always be reminded when using ellipsometry: the level of accuracy of optical properties or film thickness is highly dependent on the model; surface roughness and uniformity of films or substrates cause strong effects on the measurement results [17]. However, these difficulties can be solved. Reliable and accurate calculation can be achieved if the necessary care is taken in creating the model, defining and adhering to a clear measurement range and combining several measurements at different wavelengths or angles of incidence. Thus, the geometric limitations of conventional ellipsometers have been the primary factor preventing their use in many industrial areas.

Figure 1 shows the schematic of a standard ellipsometer in a reflection configuration. A directed beam of light with a defined polarized state is emitted by a light source, reflected by the sample in accordance with the law of reflection and detected by a receiver. A signal will only be detected if the angle and height of the transmitter and receiver are aligned in such a way that they comply with the law of reflection. This requires the angle settings of the light source and the detector to be very precisely adjusted in relation to the surface normals. The acceptable deviation of the angles of incidence is usually less than 1°. The height of the surface relative to the optical components must also be adjusted very accurately (typically better than 0.2 mm). If these conditions cannot be met, it is usually not possible to perform ellipsometric measurements because the sensor cannot receive sufficient signals. Above all, it is impossible to perform inline inspections of curved surfaces with a standard ellipsometric configuration.

3.2 Concept of retroreflex ellipsometry

At Fraunhofer IOSB, a measurement process and a prototype were developed, which overcome the geometric restrictions of ellipsometry. The principle is based on combining the transmitter and receiver in a single unit (transceiver) which is shown in Figure 2. The transmitter emits a laser beam which first reflects off the surface of the sample and then strikes a retroreflector. The polarization effect of the retroreflector used in the device is the same as an ideal mirror regardless of the angle of incidence (angular range up to approximately 30°). In contrast to a corner-cube mirror, it reflects the beam without offset back towards the sample. After reflecting off the surface of the sample again, the beam finally reaches the detector. In this configuration, the retroreflector automatically meets the reflection condition for a large range of inclination angles and heights of the test object (Figure 2(b)). In principle, it overcomes the geometric limitations of standard ellipsometers and opens the way for new industrial applications of ellipsometry. The retroreflector configuration offers the same advantages when measuring in a transmission configuration. In these applications, the use of the retroreflector ensures that the device is tolerant to the refractive powers of transparent test objects.

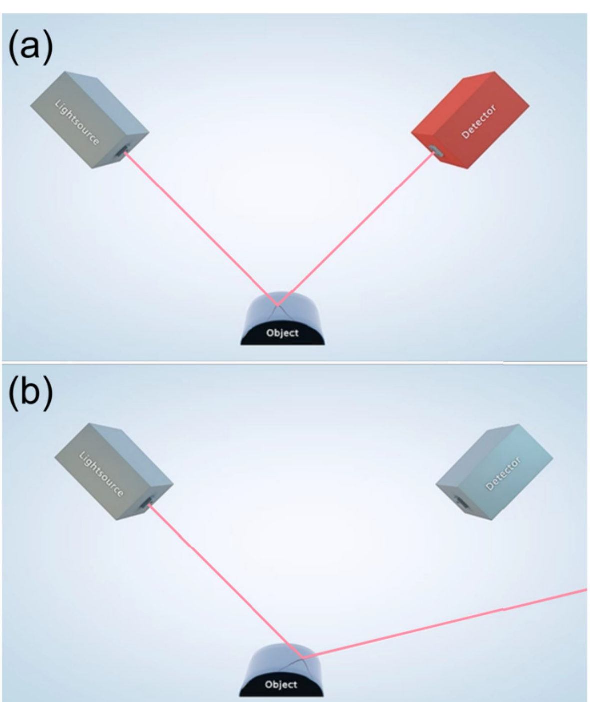

Figure 1: Beam path of a conventional ellipsometer when the reflectance condition is fulfilled (a) or not fulfilled (b).

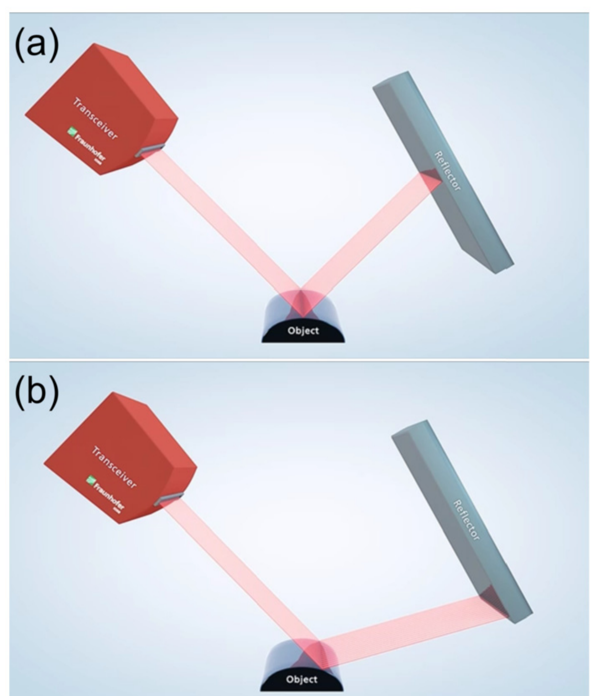

Figure 2: Realization of a laser scanner for the inline measurement of large samples. Retroreflex beam path with double reflection at the sample surface. Both beam paths (a) and (b) fulfill the reflection condition.

The evaluation of measurements from a retroreflex process differs from the setup used in standard ellipsometric evaluations in two key points:

1. The sample changes the intensity and the polarization state of the impinging light both on the way to the reflector and in the opposite direction from the reflector to the transceiver.
2. With standard ellipsometers it is essential to adjust the two angles of inclination at the sample surface very accurately to simply perform a measurement. The angle of incidence and angle of the sample in relation to the plane of incidence are therefore precisely adjusted and well known system parameters. With the retroreflex process, these angles are no longer given or known. They must be provided from a different data source (calculated separately from intensity measurements, from CAD models or additional geometrical measurements).

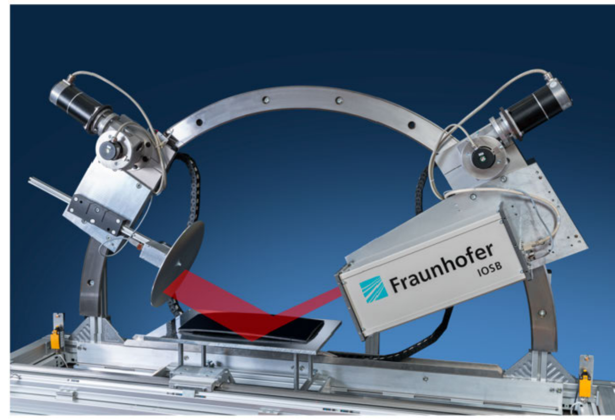

Figure 3: Prototype of the scanning retroreflex ellipsometer at Fraunhofer IOSB. The transceiver emits and receives the laser beams which are illustrated in red color. The scanning line width is about 13 cm.

4 Prototype of the scanning retroreflex ellipsometer

Figure 3 shows a prototype of the scanning retroreflex ellipsometer for ellipsometric characterization of materials over large areas in industrial processes. The prototype includes a goniometer, a scanning table, a transceiver and a retroreflector. The transmitter component of the transceiver contains a laser scanner, which scans the surface of the test object point-by-point with a laser beam and a scanning frequency of 4 MHz. A deflector unit changes the direction of the laser beam quickly that it projects a laser line, rather than a spot, onto the sample surface while ensuring that the individual light beams are aligned parallel to each other. The line scan frequency is 1 kHz. The detector component in the transceiver measures the intensities for different polarization directions. From these, it first determines the change in the polarization state caused by the illuminated element of the sample. For each point on the surface, the change in polarization of the reflected or transmitted light is measured simultaneously in several polarization channels. The measured intensities are used to determine the changes in intensity and polarization caused by the sample. Finally, the ellipsometric parameters (Ψ, Δ) can be obtained.

The measurement result is a number of polarization images which can be used to determine film thicknesses or other material properties at defined positions. In addition to positional tolerance of test objects, the prototype has a wide field of vision (line width is about 13 cm). In principle, there is no limitation to the line width in current use. It can be adapted to specific applications. Combined with the scanning table, large objects can be measured. Furthermore, the special laser focusing system produces sharp images by a small spot size (< 100 µm) within a large inspection area. Decorative defects, flaws in the material or film and inhomogeneities can be visualized and detected in high definition. One example is shown in Figure 4. In many cases (e. g., measuring film thicknesses of samples with a maximum of two films and a defined film thickness range), the parameters of the model can be determined simply by using a single wavelength. If necessary, the measurement technique can also be extended to spectral measurements since the polarization properties of the retroreflector in the visible range are virtually independent of the wavelength of the incident light.

This prototype inspection system is already suitable for use in a wide range of relevant industrial applications. The principle of the retroreflex ellipsometry allows ellipsometry to be used in general industrial applications, such as inline workpiece surface inspection, process control in roll-to-roll manufacturing processes, the measurement of drawing forces during the production of glass tubes, and film thickness measurements on painted automobile parts, coated metal surfaces or optical components.

Precise ellipsometric measurements require that the angle of incidence onto the test objects is given to a sufficient degree of accuracy for each measurement point. If absolute values are not essential (e. g., when testing homogeneity or comparing the sample with a “good” object), a knowledge of the geometry is often not required; an anal-

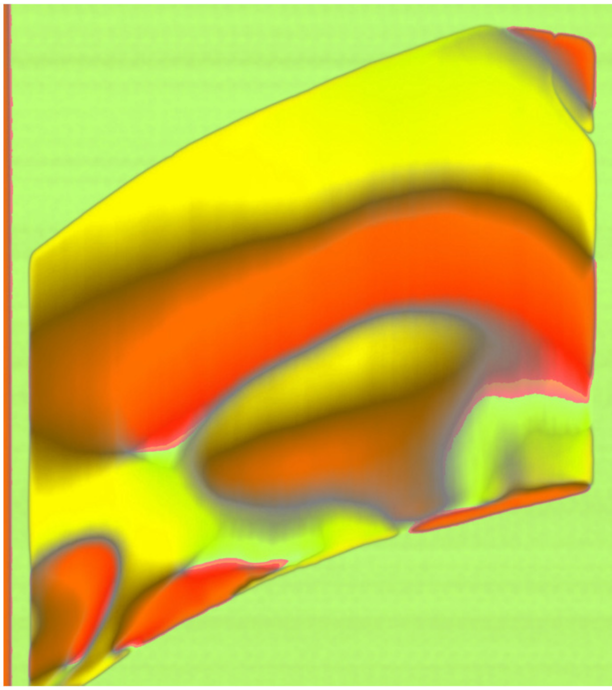

Figure 4: Polarization image of a varnished plastic test object acquired with the prototype scanner.

ysis of the homogeneity or a comparison of the acquired images is often sufficient to solve these tasks.

5 Combined reflectometric and ellipsometric characterization of dielectric substrates

5.1 Proposed method

As mentioned in the previous section, to determine absolute values, the angles of incidence onto the test objects must be constant or known to a sufficient degree of accuracy for each measurement point (e. g., from measurements or a CAD model of the test object). In this section, a simple method for measuring the angle of incidence and the refractive index of dielectric materials (substrates) is proposed. The principle bases on measurements of the reflectance R and the ellipsometric data Ψ and Δ. In general, ellipsometry measures light intensities for different states of polarization. From these measurements, the changes of the state of polarization at the sample is calculated. The reflectance can also be measured simultaneously by the same detector(s) after an absolute intensity calibration or by an additional reflectance sensor. Fresnel's equations connect R, Ψ and Δ with the refractive index n and the incident angle θ_i. From this point of view, there are two unknown parameters and two equations for R and Ψ. As shown here, it is possible to solve the equations for the refractive index n and the incident angle θ_i simultaneously and analytically. One of the advantages of this method is that the solution is in an analytical form, i. e. it is fast to calculate the result and easy to do an uncertainty analysis. Further on this method only needs a single set of measurements (R, Ψ and Δ) to determine the refractive index without prior information of the incident angle.

Figure 5 shows the refraction and reflection of a ray of light impinging from ambient material with refractive index n_i on a substrate with refractive index n_t. In this paper, the backside reflection is not considered. The polarization change can be defined as the ratio ρ of the amplitude reflection coefficients for p- and s- polarizations:

$$\rho = \frac{r_p}{r_s} = \tan \Psi e^{i\Delta}, \tag{1}$$

where $\tan \Psi$ is the ratio of the magnitude for p- and s-polarizations ($|r_p| / |r_s|$) and Δ is the phase difference ($\delta_{rp} - \delta_{rs}$). δ_{rp} and δ_{rs} are the phase changes after reflection for the p- and s- polarizations, respectively. The reflectance for natural light or unpolarized light can be expressed as

$$R = \frac{1}{2}\left(|r_p|^2 + |r_s|^2\right). \tag{2}$$

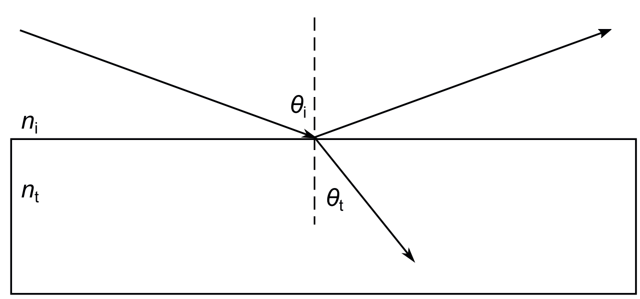

Figure 5: Reflection and refraction at a dielectric substrate.

If the substrate is an isotropic dielectric material, its extinction coefficient is 0. According to Fresnel's equations, the amplitude reflection coefficients of p- and s- polarizations are real numbers [2]. Figure 6 shows the amplitude coefficient at an air/glass interface. It is obvious that r_s is always negative, r_p is positive when Δ is 180°, and r_p is negative when Δ is 0°. The sign of r_p can be determined by the phase change Δ. Substituting $\tan \Psi = |r_p| / |r_s|$ and

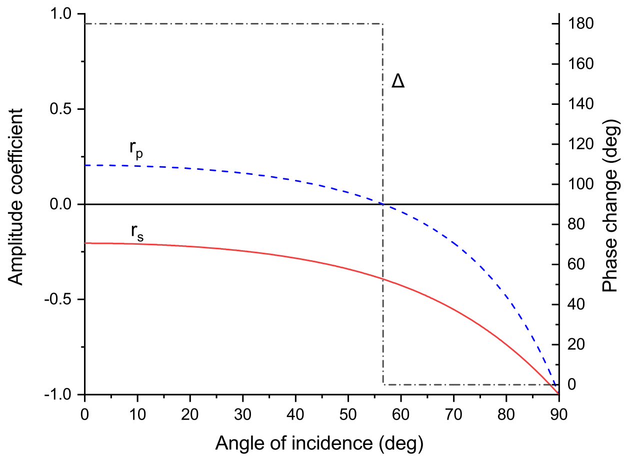

Figure 6: Amplitude coefficient r_p and r_s, and the phase change Δ at an air (n_i = 1)/glass (n_t = 1.5) interface.

the sign condition of r_p into Eq. (2), we can obtain r_p and r_s as

$$r_p = \begin{cases} \sqrt{2R}\sin\Psi, \text{if } \Delta = 180^\circ \\ -\sqrt{2R}\sin\Psi, \text{if } \Delta = 0 \end{cases}. \tag{3}$$

$$r_s = -\sqrt{2R}\cos\Psi. \tag{4}$$

The direct relation between the p- and s- polarizations and the angle of incidence [1] is shown as

$$\cos 2\theta_i = \frac{r_s^2 - r_p}{r_s - r_s r_p}. \tag{5}$$

Combining Eqs. (3) and (4) with Eq. (5), $\cos 2\theta_i$ can be rewritten as

$$\cos 2\theta_i = \begin{cases} \frac{-2\sqrt{R}\cos\Psi + \sqrt{2}\tan\Psi}{\sqrt{2} - 2\sqrt{R}\sin\Psi}, \text{if } \Delta = 180^\circ \\ \frac{-2\sqrt{R}\cos\Psi - \sqrt{2}\tan\Psi}{\sqrt{2} + 2\sqrt{R}\sin\Psi}, \text{if } \Delta = 0^\circ \end{cases}. \tag{6}$$

The angle of incidence can be directly obtained by Eq. (6) and the refractive index can be solved by Eq. (7) [2]

$$n_t = n_i \tan\theta_i \sqrt{1 - \frac{4\rho}{(1+\rho)^2)} \sin^2\theta_i}. \tag{7}$$

Using trigonometric formulas, we can rewrite $\tan\theta_i$ and $\sin\theta_i$ as:

$$\tan^2\theta_i = \frac{1 - \cos 2\theta_i}{1 + \cos 2\theta_i}. \tag{8}$$

$$\sin^2\theta_i = \frac{1}{2}(1 - \cos 2\theta_i). \tag{9}$$

Substituting Eqs. (8) and (9) to Eq. (7), the refractive index of the dielectric substrate can be expressed as

$$n_t = \begin{cases} n_i\sqrt{\frac{(\sqrt{2R}\sin\Psi+1)(\sqrt{2R}\cos\Psi+1)}{(\sqrt{2R}\sin\Psi-1)(\sqrt{2R}\cos\Psi-1)}}, \text{if } \Delta = 180^\circ \\ n_i\sqrt{\frac{(\sqrt{2R}\sin\Psi-1)(\sqrt{2R}\cos\Psi+1)}{(\sqrt{2R}\sin\Psi+1)(\sqrt{2R}\cos\Psi-1)}}, \text{if } \Delta = 0^\circ \end{cases}. \tag{10}$$

If the angle of incidence equals the Brewster angle, then $\Psi = 0$, $r_p = 0$ and $r_s = -\sqrt{2R}$. Introducing these values into Eqs. (6) and (10), we can obtain $\cos 2\theta_i = -\sqrt{2R}$ and the refractive index becomes

$$n_t = n_i\sqrt{\frac{1+\sqrt{2R}}{1-\sqrt{2R}}}. \tag{11}$$

5.2 Evaluation of the proposed method

In order to verify the proposed method, the reflectometric and the ellipsometric measurements presented by Hazebroek and Visser [9] are taken. They used a laser interferometric ellipsometer to measure the ellipsometric parameters and the reflectance of a silica disc (Heraues Ultrasil). Table 1 shows the experimental data and the calculated data using the nominal refractive index at two different angles of incidence. The same data in Table 1 is used to verify the proposed method. Here we assume that the phase difference Δ of the measurements is zero. In Table 2, two experimental results and two theoretical values are calculated by the proposed method. The calculation results are almost the same as the theoretical values. Only one result has 0.0001 difference in the refractive index. The reason could be the rounding error or the resolution of the experiment data. For the calculation of experimental results, the

Table 1: Experimental data and calculated parameters for silica whose refractive index is 1.4593 at a wavelength of 568.1 nm. The table is reproduced from [9], where $R_\parallel = R_p$, $R_\perp = R_s$ and $R = \frac{1}{2}(R_\parallel + R_\perp)$.

	Angle of incidence	Ellipso-/reflectometry					Associated optical constants	
	θ_i	Ψ	Δ	$R_\parallel$	$R_\perp$	R	n	k
Exp. 1	69.78°	21.31°	−0.03°	0.0397	0.2737	0.1567	1.4595	0.0004
Theory 1	–	21.32°	0°	0.0424	0.2783	0.1604	1.4593	0
Exp. 2	74.77°	27.84°	0.05°	0.1010	0.3683	0.2347	1.4590	0.0011
Theory 2	–	27.83°	0°	0.1047	0.3757	0.2402	1.4593	0

Table 2: Calculation results of Table 1 by the proposed method.

	Angle of incidence θ_i	Refractive index n	$\Delta\theta_i$	Δn
Evaluation of Exp. 1	69.62°	1.4508	−0.16°	−0.0087
Evaluation of Theory 1	69.78°	1.4592	0°	0.0001
Evaluation of Exp. 2	74.61°	1.4487	−0.16°	−0.0103
Evaluation of Theory 2	74.77°	1.4593	0°	0

maximum differences of the angle of incidence and the refractive index are 0.16° and 0.0103. These results show a very satisfactory agreement and prove the correctness of the derived equations. The most probable error source in the set of measurements is the reflectance. It is smaller than the theoretical value. The reason could be an effect of surface roughness which might cause a small amount of non-specularly scattered light. Also, the experimental result of the phase difference Δ is not zero which differs from the nominal value. For more details, see [9].

In this section, a simple method has been proposed for determining the angle of incidence and the refractive index of dielectric substrates simultaneously by evaluation of reflectance and ellipsometric data. The feasibility of the method has been proven by using published experimental data. The advantages of the method are:

1. The angle of incidence and the refractive index are determined analytically by a single set of measurements of reflectance and ellipsometric data.
2. An absolute intensity calibration is sufficient to extend existent ellipsometers with this method.
3. The uncertainties of the incident angle and the refractive index can also be determined analytically.

5.3 Potential applications

The proposed method can be used in retroreflex ellipsometry to evaluate the angle of incidence and the index of refraction of dielectric substrates. Moreover, this method can be extended to other applications, e. g., the calibration process of the angle of incidence for goniometers in ellipsometers. In conventional ellipsometry, the angle of incidence is measured by the goniometer. The calibration of the goniometer is necessary for minimizing the angular error. Auxiliary optics (e. g., autocollimators) are usually used for precise alignment of goniometers. However, it is difficult to apply the direct measurement of the angle of incidence in in-line and in situ ellipsometers due to the space limit or the inaccessibility of a vacuum chamber. Therefore, indirect measurement of the angle of incidence might be helpful for in-line and in situ ellipsometers. By the proposed method, the angle of incidence can be determined indirectly with a dielectric substrate. In addition, the prior knowledge of the surface orientation and the index of refraction of that dielectric substrates is not necessary. These features could provide an easy and fast calibration method for goniometers in general, in-line and in situ ellipsometers.

Another application could be three-dimensional shape measurements of dielectric substrates. By the proposed method and a determination of the tilt angle [3], surface orientation can be obtained. Then the shape of the sample can be reconstructed. The advantage of this method is that the optical properties and the shape of the sample can be measured at the same time with one device, which reduces costs and measurement time.

6 Summary

The principle of the retroreflex ellipsometry allows ellipsometry to be used in many industrial applications. The prototype of a laser scanning retroreflex ellipsometer can detect changes in polarization for test objects with flat and curved surfaces at a high resolution, over a large field of measurement and in inline processes. As well as changes in polarization, it can also measure changes of intensity (transmittance or reflectance). Defects on a surface scatter the light in all directions and show up as dark spots on the image. This occurs with flaws such as scratches, holes and cracks. Therefore retroreflex ellipsometry is in principle capable of performing inline measurements to determine the perfection of the test object regarding aesthetic or functional quality criteria as well as the material quality of test objects or coatings. As shown here, the combination of retroreflex ellipsometry and retroreflex reflectometry enables precise measurements of the refractive index and the angle of incidence for dielectric substrates. Together with a determination of the tilt angle, it allows the characterization of material and geometry of freeform optics. By overcoming the geometric restrictions of existing setups, ellipsometric measurements can now be used comprehensively in many industrial production processes for the first time.

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