# An Overview of Ellipsometric Measurements for Nonplanar Surfaces

Chia-Wei Chen

Vision and Fusion Laboratory Institute for Anthropomatics Karlsruhe Institute of Technology (KIT), Germany chia-wei.chen@kit.edu

Technical Report IES-2019-09

### Abstract

Ellipsometry is an optical method used for characterizing materials and thin films. The principle of ellipsometry is that it measures polarization changes at a sample in a reflection or transmission configuration. However, the shape of the sample is limited to flat or nearly flat surfaces because ellipsometry is sensitive to the angle of incidence, tilt angle and the sample position (height). Even slight misalignment of the sample might lead to significant experimental errors. For large misalignment, the detector of the ellipsometer is not feasible to receive sufficient signals. There have been a few approaches for characterizing nonplanr surfaces by ellipsometry. This report gives an overview of these approaches for ellipsometric measurements of nonplanar surfaces.

# 1 Introduction

Ellipsometry is an optical technique for characterization of materials and thin films. The main features of ellipsometry are high precision (thickness from

a few Å to several tens of microns), nondestructive measurement, and wide applications. The principle of ellipsometry is that it measures polarization changes at a sample in a reflection or transmission configuration. Fig. 1.1 shows the principle of reflection ellipsometry. The incident light is linearly polarized. After the reflection from the substrate, the reflected light becomes elliptically polarized. The Fresnel equations describe the interaction of light (electromagnetic waves) and materials. The polarization changes can be defined as the ratio  $\rho$  of the amplitude reflection coefficients for p- and s- polarizations [1]:

$$\rho = \frac{r_p}{r_s} = \tan \Psi e^{i\Delta},\tag{1.1}$$

where  $\Psi$  and  $\Delta$  present amplitude ratio and phase difference. Ellipsometry technique can be applied to many scientific and industry fields, e.g., semiconductor, chemistry, display industry and biomaterials [7].

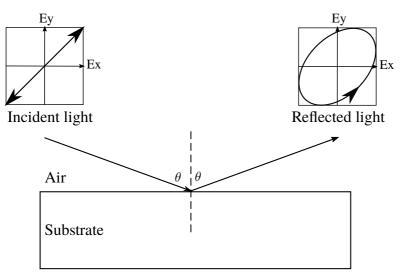
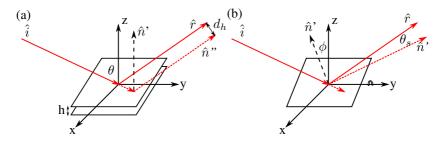


Figure 1.1: Measurement principle of ellipsometry.

In conventional ellipsometers, samples are limited to a planar shape because ellipsometry is sensitive to the angle of incidence (AOI), tilt angle and the sample

position (height). Even slight misalignment of the position and orientation of the sample might lead to significant experimental errors. For large misalignment, the detector of the ellipsometer is not feasible to receive sufficient signals. For nonplanar surfaces, the beam path of reflected or transmitted light is changed because of the surface shape. In order to solve this problem, different methods have been proposed for nonplanar surfaces. In this paper, we will review and compare these approaches in the configuration of reflection ellipsometry.

#### **2** Surface orientation in reflection ellipsometry



**Figure 2.1**: Definition of the surface orientation. (a) An offset h along the surface normal  $\hat{n}$ . (b) The surface rotates around the y-axis.

Fig. 2.1(a) shows a planar surface defining the xy-plane. The z-axis (0, 0, 1) is the surface normal  $\hat{n}$ . The hat is denote as a unit vector. If the incident beam  $\hat{i}$ is on the yz plane and the incident angle is  $\theta$ , the incident beam is expressed as:  $(0, \sin \theta, -\cos \theta)$ . The reflected beam  $\hat{r}$  can be defined as:  $(0, \sin \theta, \cos \theta)$ . The relationship between  $\hat{n}$ ,  $\hat{i}$ , and  $\hat{r}$  is shown as [11]:

$$\hat{r} = \hat{i} - 2(\hat{i} \cdot \hat{n})\hat{n}. \tag{2.1}$$

The angle of incidence  $\theta$  is determined by the surface normal  $\hat{n}$  and the incident beam  $\hat{i}$  as:

$$\theta = \cos^{-1} - \hat{i} \cdot \hat{n}. \tag{2.2}$$

If the surface has an offset h along the surface normal  $\hat{n}$  as shown in Fig. 2.1(a), it will cause an offset  $d_h$  of the reflected beam as:

$$d_h = 2h\sin\theta \tag{2.3}$$

For an incident angle of  $70^{\circ}$  and an offset of 1 mm, the offset  $d_h$  is about 1.88 mm.

Fig. 2.1(b) illustrates a surface rotates around the y-axis. The surface normal of the sample becomes  $\hat{n}' = (\sin \phi, 0, \cos \phi)$ . Using Eq. 2.2, we can easily compute the angle of incidence  $\theta'$  and the reflected beam  $\hat{r}'$  after the rotation as:

$$\cos\theta' = \cos\theta\cos\phi, \tag{2.4}$$

$$\hat{r}' = (\cos\theta\sin 2\phi, \sin\theta, \cos\theta\cos 2\phi). \tag{2.5}$$

The included angle  $\theta_s$  between the original reflected beam  $\hat{r}$  and the reflected beam  $\hat{r}'$  after tilting can be calculated by the product rule from:

$$\cos\theta_s = \sin^2\theta + \cos^2\theta\cos 2\phi. \tag{2.6}$$

For an incident angle of  $70^{\circ}$ , if a surface tilts  $5^{\circ}$  around y-axis, it will produce an angle deviation by  $3.4^{\circ}$  for the detector. If the distance between the surface and the detector is 200 mm, it will induce an offset of 11.9 mm.

From the above calculation results, surface offset and tilt produce a significant offset for the detector, which will degrade the measurement accuracy. Therefore, special optical designs, compensation methods and precision alignment are necessary for ellipsometric measurements of nonplanar surfaces.

# 3 Ellipsometric measurements for nonplanar surfaces

There have been a few approaches for characterizing nonplanar surfaces by ellipsometry. These approaches can be categorized into three types: combination of topometry and ellipsometry, polarization model for azimuth deviations, and return-path ellipsometry with special reflectors. In this section, the basic principles and the main features of these approaches will be introduced.

#### 3.1 Combination of topometry and ellipsometry

In order to simultaneously determine the topometry and optical constants of surfaces, the combinations of ellipsometry and topometric measurements are proposed, e.g., laser interferometry [16], microscopic fringe projection [15] and white light interferometry [14]. A high numerical aperture (NA) microscope objective is used to collect the reflected light, which is shown in Fig. 3.1. The topometric measurements can measure heights in relative to a plane of reference and ellipsometric measurements can measure the optical constants or film thicknesses. The common feature of these configurations is the off-axis focusing method which can provide tilted irradiation on the surface, high lateral resolution, and collect the reflected light from the nonplanar surface. High NA microscope objectives can measure steep inclinations of surfaces. However, the working distance is short, e.g, an objective with a NA of 0.8 has a working distance of 1 mm.

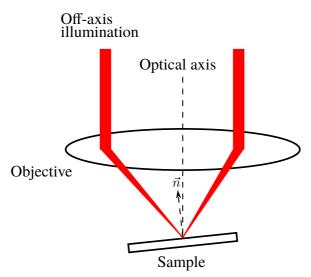


Figure 3.1: Internal focusing and off-axis illumination with a tilted sample.

In contrast to the internal focusing, Wirth [21] proposed micro-deflectionellipsometry to combine topometric and ellipsometric measurements , which is shown in Fig. 3.2. He used a lens system to collect the reflected light for the polarization state generator (PSG), and a beamsplitter to split the reflected light to a position sensitive detector (PSD) and an ellipsometric detector. The PSD can determine the surface orientation and the ellipsometric parameters can be obtained by the ellipsometric detector. In order to receive evaluable signals from the curved surface, the diameter of the first lens should have a large aperture. Therefore, Fresnel lenses are used in the optical system. Compared to the internal focusing, this configuration has a higher working distance of 100 mm.

#### 3.2 Polarization model for azimuth deviations

Lee and Chao [13] found the azimuth deviation of the polarizer is the same as the deviation of the surface normal in a calibrated rotating-analyzer ellipsometer. The relationship can be described by Mueller matrices [1]:

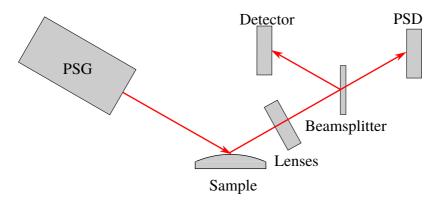


Figure 3.2: Combination of topometry (PSD) and ellipsometry (adapted from Wirth [21]).

$$\mathbf{M}_{meas} = \mathbf{M}_A \cdot \mathbf{R}(A) \cdot \mathbf{M}_{sample} \cdot \mathbf{R}(-P) \cdot \mathbf{M}_P, \qquad (3.1)$$

where  $\mathbf{M}_{meas}$ ,  $\mathbf{M}_{sample}$ ,  $\mathbf{M}_A$ ,  $\mathbf{M}_P$  and  $\mathbf{R}$  are the Mueller matrices of the measured matrix, the nondepolarizing isotropic sample, the analyzer, the polarizer and the rotation matrix, respectively. *P* and *A* of the rotation matrix  $\mathbf{R}$  represent the rotation angle of the polarizer and the analyzer. They used Eq. 3.1 and a three-intensity imaging ellipsometer to measure the surface topography and the coating thickness of a lens.

Neuschaefer-Rube and Holzapfel [19] proposed a method to measure surface geometry and material distribution. They used the internal focusing to collect the reflected beam from the curved surface, which is introduced in section 3.1. Despite of the similar configuration, the surface inclinations can be determined directly by the polarization model without other topometric measurement methods. The polarization model is expressed as:

$$\mathbf{M}_{meas} = \mathbf{R}(\theta_{out}) \cdot \mathbf{R}(-\phi) \cdot \mathbf{M}_{sample} \cdot \mathbf{R}(\phi) \cdot \mathbf{R}(\theta_{in}), \quad (3.2)$$

where  $\theta_{in}$ ,  $\theta_{out}$  and  $\phi$  are the azimuthal rotation angles on the principle plane of focusing optics. The angle of incidence and the surface orientation can be obtained by the eight-zone-measurement algorithm. After the scanning for the whole surface, the profile can be reconstructed from the surface inclination (gradient data).

Johs and He [12] used a return-path ellipsometer to measure samples which have a wobble effect. The configuration of return-path ellipsometry will be introduced in Fig. 3.3. They established a Mueller matrix model to describe the measurement system. The model is shown as:

$$\mathbf{M}_{meas} = \mathbf{R}(rec) \cdot \mathbf{M}_{sample} \cdot \mathbf{M}_{mirror} \cdot \mathbf{M}_{sample} \cdot \mathbf{R}(src), \quad (3.3)$$

where rec and src are the rotation angles of the receiver and the source. They compensated a  $\pm 0.8^{\circ}$  substrate wobble and reduced the signal variation to less than 2%.

Li et al. [17] considered the effect of the incident plane deviation and proposed a Mueller matrix model to describe the Mueller matrix of the tilt surface as:

$$\mathbf{M}_{meas} = \mathbf{R}(-\alpha) \cdot \mathbf{M}_{sample} \cdot \mathbf{R}(\alpha). \tag{3.4}$$

They believed the two rotation have the same absolute values but different signs. By using Mueller matrix ellipsometry, they successfully measured the oxide layer thickness and the curvature radius for a spherical lens.

Duwe et al. [6] modified the Muller matrix model of Li et al. because of a significant mismatch at larger tilt angles. The modified model is described as:

$$\mathbf{M}_{meas} = \mathbf{R}(-\delta) \cdot \mathbf{M}_{sample} \cdot \mathbf{R}(\gamma), \qquad (3.5)$$

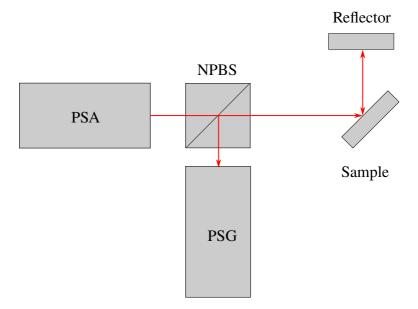
where  $\delta$  and  $\gamma$  are rotation angles of the Mueller rotation matrix. In contrast to the model of Li et al., they assumed the two rotation angles have different signs and values. They used a spectroscopic imaging ellipsometer to measure single-layer coating on a microlens.

#### 3.3 Return-path ellipsometry

In return-path ellipsometry, the light beam reflected from the surface is reflected back to the same position from the surface by a mirror [20, 2]. Fig. 3.3 illustrates the schematic of return-path ellipsometry. The advantages of this configuration are simple construction, suitable for process monitoring, and higher sensitivity to the optical properties of surfaces than conventional ellipsometers. Please refer to [3] for more details.

In most semiconductor process, samples usually need to rotate to obtain uniform layers, e.g., plasma-enhanced chemical vapor deposition and epitaxial growth process. The rotation of samples inevitably produces a wobble effect because the rotation axis and the surface normal of the sample are not parallel. As mentioned in section 2, ellipsometry is very sensitive to the angle of incidence and the sample position. In order to obtain accurate measurements, Haberland et al. [9] used return-path ellipsometry and replaced the plane mirror by using a spherical mirror. In geometry ray tracing, every ray which passes the vertex of the spherical mirror is reflected back along the original path. This configuration can effectively reduce the error from the angle deviation for sample rotation and sample wobbling during the manufacturing process.

In order to solve the alignment problem between the sample and the detector, Hartrumpf and Negara [10] developed a laser scanner to overcome this limitation



**Figure 3.3**: Configuration of return-path ellipsometry, where PSA, PSG and NPBS are polarization state generator, polarization state analyzer and non-polarizing beamsplitter, respectively.

by a retroreflector (retroreflective sheet). The principle is based on return-path ellipsometry which is shown in 3.3. They used a retroreflector as a reflector. A retroreflector can return the light beam from the sample back on the same beam path with only a phase difference of  $180^{\circ}$ . In other words, the polarization effect is the same as an ideal mirror. In this configuration, the alignment condition for the sample and the detector is fulfilled at an angle deviation up to  $30^{\circ}$ . Chen et al. used this concept to develop a ellipsometer and measured the ellipsometric parameters and the refractive index for nonplanar surfaces [4, 5].

# 4 Discussion and comparison

For ellipsometric measurements of nonplanar surfaces, combination of topometry and ellipsometry is a straightforward method. This method can achieve very high lateral resolution (about  $2.8 \,\mu\text{m}$  in [19]). However, the hardware of topometry will increase the complexity of the whole system, especially for the system alignment and the calibration. In addition, these methods use a focused beam. In order to acquire accurate results, correct focusing planes of the measurement beam are important. Auto focusing methods are applied in these approaches. For the measurement of the whole surface, vertical and xy scanning for every point are necessary, which is very time-consuming.

Polarization models for azimuth deviations provide another solution for surface geometry. This method can be easily applied to conventional ellipsometers without extra hardware. Nonetheless, the range of topometric measurements is limited to a small range because the polarization characteristic of the analyzer (waveplate) is sensitive to the incident angle [8]. Waveplates are constructed by birefringent materials and designed for a normal incident angle. Thus, the retardance of a waveplate will change when the incident angle is not normal. Large incident angles for the waveplate will induce significant errors of the retardance. On the other hand, if the sample is tilted, according to the calculation in 2, the beam offset from the detector is large. Adjustment of the position for the detector is necessary and also time-consuming.

Return-path ellipsometry has a high sensitivity of optical properties of materials due to the double reflection from the sample. Special reflectors (spherical mirror and retroreflector) can achieve ellipsometric measurements for nonplanar surfaces. However, the disadvantages of this configuration are the need for a high power light source and the polarization distortion induced by the non-polarizing beamsplitter. The non-polarized beamsplitter loses a large amount of power of the light source (more than 75%). Moreover, the non-polarized beamsplitter is not an ideal component in polarization optics [18, 22]. Therefore, the calibration of the beamsplitter is necessary.

### 5 Summary

In this report, we have introduced different approaches for ellipsometric measurements of nonplanar surfaces including the principles and the main features. Each approach has its own advantages, disadvantages and suitable application fields. Conventional ellipsometers can only measure samples with flat or nearly flat surfaces. However, there is an urgent need for ellipsometric measurements of nonplanar surfaces in the market, e.g., lens coatings and varnish layer on metallic objects. Further research should be conducted in theory and hardware development for needs of industries.

### References

- [1] R. M. A. Azzam and N. M. Bashara. *Ellipsometry and polarized light*. Amsterdam and Oxford: North-Holland, 1977. ISBN: 9780444870162.
- R.M.A. Azzam. "Return-path Ellipsometry and a Novel Normal-incidence Null Ellipsometer (NINE)". In: *Optica Acta: International Journal of Optics* 24.10 (1977), pp. 1039–1049. ISSN: 0030-3909. DOI: 10.1080/ 713819411.
- [3] Chia-Wei Chen. "An Overview of Return-Path Ellipsometry". In: Proceedings of the 2018 Joint Workshop of Fraunhofer IOSB and Institute for Anthropomatics, Vision and Fusion Laboratory. Ed.: J. Beyerer, M. Taphanel. Vol. 40. Karlsruher Schriften zur Anthropomatik / Lehrstuhl für Interaktive Echtzeitsysteme, Karlsruher Institut für Technologie ; Fraunhofer-Inst. für Optronik, Systemtechnik und Bildauswertung IOSB Karlsruhe. KIT Scientific Publishing, Karlsruhe, 2019, pp. 1–10. ISBN: 978-3-7315-0936-3.
- [4] Chia-Wei Chen et al. "Measurement of ellipsometric data and surface orientations by modulated circular polarized light / Messung von ellipsometrischen Daten und Oberflächenorientierungen durch moduliertes zirkular polarisiertes Licht". In: *tm - Technisches Messen* 86.s1 (2019), pp. 32–36. ISSN: 2196-7113. DOI: 10.1515/teme-2019-0047.

- [5] Chia-Wei Chen et al. "Retroreflex ellipsometry for isotropic substrates with nonplanar surfaces". In: *Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena* 38.1 (2020), p. 014005. ISSN: 2166-2746. DOI: 10.1116/1.5121854.
- [6] Matthias Duwe et al. "Thin-film metrology of tilted and curved surfaces by imaging Mueller-matrix ellipsometry". In: *Journal of Vacuum Sci*ence & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena 37.6 (2019), p. 062908. ISSN: 2166-2746. DOI: 10.1116/1.5122757.
- [7] Hiroyuki Fujiwara. Spectroscopic ellipsometry: Principles and applications. Chichester, England and Hoboken, NJ: John Wiley & Sons, 2007.
  ISBN: 9780470060186. DOI: 10.1002/9780470060193.
- [8] Honggang Gu et al. "Study of the retardance of a birefringent waveplate at tilt incidence by Mueller matrix ellipsometer". In: *Journal of Optics* 20.1 (2017), p. 015401. ISSN: 2040-8986. DOI: 10.1088/2040-8986/aa9b05. URL: https://iopscience.iop.org/article/10.1088/2040-8986/aa9b05/pdf.
- [9] K. Haberland et al. "Ellipsometric and reflectance-anisotropy measurements on rotating samples". In: *Thin Solid Films* 313-314 (1998), pp. 620– 624. ISSN: 00406090. DOI: 10.1016/S0040-6090(97)00897-3.
- [10] Matthias Hartrumpf and Christian Negara. *Configurable retro-reflective* sensor system for the improved characterization of the properties of a sample. WO/2017/207681. 7.12.2017.
- [11] Eugene Hecht. Optics. 4th ed. Reading Mass.: Addison-Wesley, 2002. ISBN: 9780805385663.
- Blaine Johs and Ping He. "Substrate wobble compensation for in situ spectroscopic ellipsometry measurements". In: *Journal of Vacuum Science & Technology B, Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena* 29.3 (2011), p. 03C111. ISSN: 2166-2746. DOI: 10.1116/1.3555332.

- Kan Yan Lee and Yu Faye Chao. "The Ellipsometric Measurements of a Curved Surface". In: *Japanese Journal of Applied Physics* 44.7L (2005), p. L1015. ISSN: 1347-4065. DOI: 10.1143/JJAP.44.L1015. URL: http: //iopscience.iop.org/article/10.1143/JJAP.44.L1015/pdf.
- [14] K. Leonhardt. "Ellipso-Height Topometry, EHT: Extended topometry of surfaces with locally changing materials". In: *Optik - International Journal for Light and Electron Optics* 112.9 (2001), pp. 413–420. ISSN: 0030-4026. DOI: 10.1078/0030-4026-00079.
- [15] K. Leonhardt, U. Droste, and H. J. Tiziani. "Topometry for locally changing materials". In: *Optics Letters* 23.22 (1998), p. 1772. ISSN: 1539-4794. DOI: 10.1364/0L.23.001772.
- K. Leonhardt, H.-J Jordan, and H. J. Tiziani. "Micro-Ellipso-Height-Profilometry". In: *Optics Communications* 80.3-4 (1991), pp. 205–209.
  ISSN: 00304018. DOI: 10.1016/0030-4018(91)90251-8.
- [17] Weiqi Li et al. "Characterization of curved surface layer by Mueller matrix ellipsometry". In: *Journal of Vacuum Science & Technology B*, *Nanotechnology and Microelectronics: Materials, Processing, Measurement, and Phenomena* 34.2 (2016), p. 020602. ISSN: 2166-2746. DOI: 10.1116/1.4943952.
- [18] Yeng-Cheng Liu, Yu-Lung Lo, and Chia-Chi Liao. "Compensation of non-ideal beam splitter polarization distortion effect in Michelson interferometer". In: *Optics Communications* 361 (2016), pp. 153–161. ISSN: 00304018. DOI: 10.1016/j.optcom.2015.09.099.
- [19] Ulrich Neuschaefer-Rube and Wolfgang Holzapfel. "Simultaneous measurement of surface geometry and material distribution by focusing ellipsotopometry". In: *Applied Optics* 41.22 (2002), p. 4526. ISSN: 0003-6935. DOI: 10.1364/A0.41.004526.
- [20] H. M. O'Bryan. "The Optical Constants of Several Metals in Vacuum\*". In: JOSA 26.3 (1936), pp. 122–127. DOI: 10.1364/JOSA.26.000122. URL: https://www.osapublishing.org/viewmedia.cfm?uri=josa-26-3-122&seq=0.

- [21] Frank Wirth. "Zur Erfassung von form- und materialbedingten Oberflächenstrukturen mit Mikro-Deflexions-Ellipsometrie". Kassel., Univ., Diss., 2008. PhD thesis. 2008. URL: https://kobra.bibliothek.unikassel.de/handle/urn:nbn:de:hebis:34-2008020120181.
- [22] Song Zhang et al. "Characterization of beam splitters in the calibration of a six-channel Stokes polarimeter". In: *Journal of Optics* 20.12 (2018), p. 125606.