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Ellipsometry — Principles

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Contents

Page

Foreword iv

Introduction v

1 Scope 1

2 Normative references 1

3 Terms, definitions, symbols and abbreviated terms 1

3.1 Terms and definitions 1

3.2 Symbols and abbreviated terms 1

4 Experimental boundary conditions with respect to the sample 2

5 Experimental boundary conditions with respect to the measurement 3

6 Model-correlated boundary conditions of the simulation 4

7 Basic models 4

7.1 General 4

7.2 Bulk material (case 1 of application) 5

7.3 Transparent single layer (case 2 of application) 5

7.4 Semi-transparent single layer (case 3 of application) 5

7.5 Multiple layers and periodic layers (case 4 of application) 5

7.6 Effective materials (case 5 of application) 5

8 Raw data 5

9 Verification of correct adjustment of the device 5

9.1 Straight line measurement 5

9.2 Simple measurement of angles 6

9.2.1 Measurement on a known sample, e.g. SiO_2/Si, with fitting of the angle of incidence 6

9.2.2 Measurement of the Brewster's angle of water, of a solvent or of technical glass 8

10 Verification of the device regarding correct calibration 9

11 Test report 9

Annex A (informative) **Mathematical and physical principles of ellipsometry** 10

Bibliography 15

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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This document was prepared by Technical Committee ISO/TC 107, *Metallic and other inorganic coatings*.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

The ellipsometry measuring method is a phase-sensitive reflection technique using polarized light in the optical far-field. Over a long time, ellipsometry has been established as a non-invasive measuring method in the field of semiconductor technology — especially within the integrated production — in the first instance as a single-wavelength, then as a multiple-wavelength and later as a spectroscopic measuring method.

By means of ellipsometry, optical or dielectric constants of any material as well as the layer thicknesses of at least semi-transparent layers or layer systems can be determined. Ellipsometry is an indirect measuring method, the analysis of which is based on model optimization. The measurands, which differ according to the procedural principle, are converted into the ellipsometric factors Ψ (Psi, amplitude information) and Δ (Delta, phase information), based on which the physical target figures of interest (optical or dielectric constants, layer thicknesses) will then be determined by means of a parameterized fit.

Ellipsometry shows a high precision regarding the ellipsometric transfer quantities Ψ and Δ, which can be equivalent to a layer thickness sensitivity of 0,1 nm for ideal layer substrate systems. As a result, the measuring method can verify even the slightest discrepancies in the surface characteristics. This is closely linked to the homogeneity and the isotropy of the material surface. In order to achieve high precision, carrying out measurements at the exact same measuring point is a prerequisite for inhomogeneous materials. The same applies to the orientation of the incident plane relative to the material surface for anisotropic materials.

The absolute accuracy, e.g. of layer thickness values, substantially depends on the quality of the chosen model for describing the material surface. For ideal layer substrate systems, such as SiO_2 (ideal transparent layer) on a Si wafer (nearly atomically smooth substrate surface with homogeneous and isotropic material properties), the accuracy of the layer thickness can indeed reach the precision values, since the model describes the reality of the layer substrate system in an ideal manner. For inhomogeneous, anisotropic, contaminated, multi-component, damaged, imperfect or rough surfaces or layers, the accuracy of the layer thickness determination can be significantly lower and generally depends on the quality of the chosen model.

Despite these limitations, ellipsometry is a powerful procedure, which either enables material fingerprints (without modelling) or which allows a model-based determination of optical and dielectric constants (to the nearest 0,001) or of layer thicknesses (to the nearest 0,1 nm) within a broad layer thickness range of approximately 0,1 nm up to approximately 10 µm (in special cases exceeding 100 µm).

Ellipsometry — Principles

1 Scope

This document specifies a method for determining optical and dielectric constants in the UV-VIS-NIR spectral range as well as layer thicknesses in the field of at-line production control, quality assurance and material development through accredited test laboratories.

It is applicable to stand-alone measuring systems. The presentation of the uncertainty of results conforms to ISO/IEC Guide 98-3.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO/IEC Guide 98-3, *Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

3 Terms, definitions, symbols and abbreviated terms

3.1 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

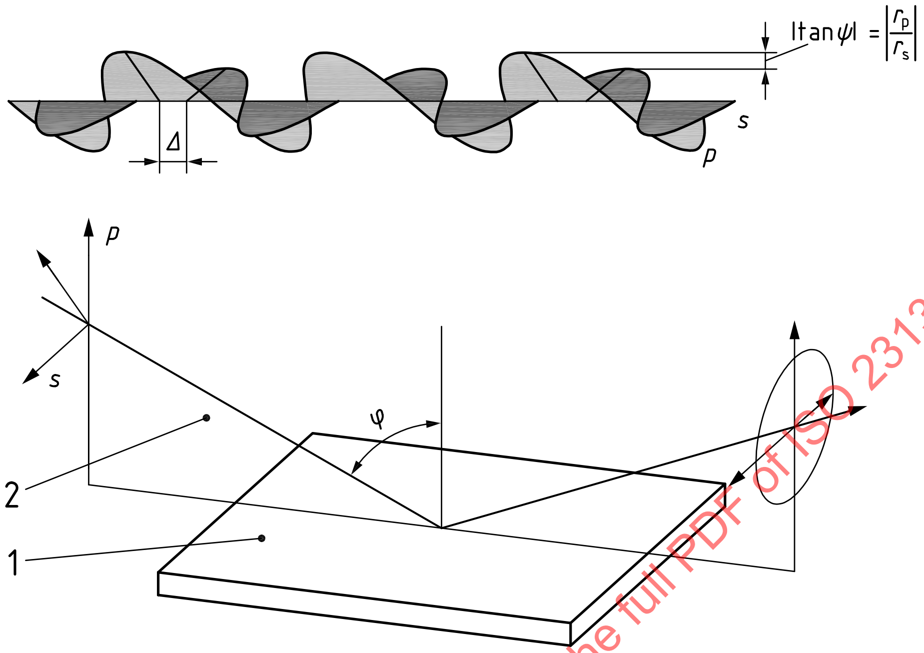
— IEC Electropedia: available at http://www.electropedia.org/

3.2 Symbols and abbreviated terms

Symbol or abbreviated term	Description
P	polarizer
C	compensator
S	sample
A	analyzer
POI	plane of incidence of light, formed by the normal to the surface and the direction of propagation of the incident light
POP	plane of polarization of light, formed by the electric field vector and the direction of propagation of the incident light
Ψ, Δ	ellipsometric transfer quantities Psi and Delta, which serve as raw data to be stored, e.g. in accordance with ISO/IEC 17025
φ	angle of incidence between the incident light wave and the axis of incidence
d	layer thickness

4 Experimental boundary conditions with respect to the sample

Figures 1 and 2 schematically represent an ellipsometric measurement as a phase-sensitive reflection technique using polarized light; both under photo-optical aspects (see Figure 1) as well as under metrological aspects (see Figure 2).



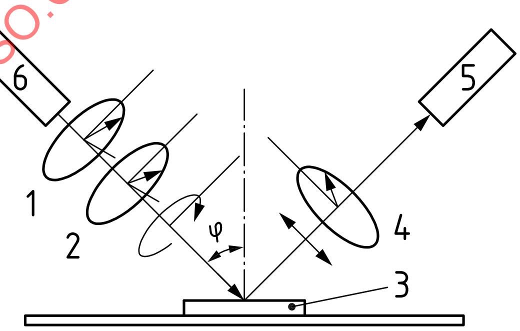
Key

1 sample

2 POI

φ angle of incidence

Figure 1 — Schematic representation of the optical path/polarization state before and after reflection (substrate surface, axis and angle of incidence, optical path/light wave, s- and p-polarization)



Key

1 polarizer

2 compensator

3 sample

4 analyser

5 detector

6 light source

Figure 2 — Schematic representation of the metrological arrangement (light source, P-C-S-A configuration)

The following experimental boundary conditions with respect to the sample should be agreed upon in advance and, if relevant, be documented in the test report:

— determine/specify the measuring point (evaluation of homogeneity) and the sample orientation (evaluation of isotropy);

— surface condition: take a micrograph of the surface if necessary;

— surface topography: if necessary, measure the surface roughness;

— further sample properties to be considered or corrected:

  — curved and wedged samples;

  — influence of backside reflection (for transparent samples), if present;

  — surface as-delivered or cleaned;

  — fixation of the sample.

5 Experimental boundary conditions with respect to the measurement

The following experimental boundary conditions with respect to the measurement should be agreed upon in advance and, if relevant, be documented in the test report:

— indication of whether an imaging ellipsometer or a mapping ellipsometer (manual or automatic) is concerned;

— for imaging ellipsometers the following factors are relevant: resulting size of the measuring field/of the region of integration [FOI (field of illumination: sample surface that is illuminated by the incident light), FOV (field of view: sample surface within the FOI from which the light collected by the detector originates), ROI (region of interest: sample surface within the FOV that is relevant for the measurement)];

— for mapping ellipsometers the following factors are relevant: resulting size of the measuring field/of the region of integration [FOI (field of illumination: sample surface that is illuminated by the incident light), FOA (field of analysis: sample surface within the FOI from which the light collected by the detector originates)];

— ellipsometer configurations: [P-S-A, P-C-S-A, P-S-C-A or P-C-S-C-A];

— ellipsometer principle [RAE (rotating analyser ellipsometer), RPE (rotating polarizer ellipsometer), PME (phase modulated ellipsometer), RCE (rotating compensator ellipsometer), NE (nulling ellipsometer), SSE (step scan ellipsometer), RSE (referenced spectral ellipsometer), etc.];

— ellipsometry class [SWE (single-wavelength ellipsometry), MWE (multiple-wavelength ellipsometry), SE (spectroscopic ellipsometry)];

— spectral range used and resulting spectral resolution, especially dependent on the light source and the spectrometer used;

— angle of incidence, multiple-angle measurement for the verification of the model, preferably/at least for two substantially different angles of incidence;

— orientation of sample on the sample stage;

— position of the FOV or FOA on the sample;

— alignment of the sample relative to the plane of incidence (POI) and/or relative to the plane of polarization (POP).

6 Model-correlated boundary conditions of the simulation

The following boundary conditions with respect to the simulation shall be agreed upon in advance and, if relevant, be documented in the test report:

— definition of the ellipsometric model (substrate material, roughness, layer architecture, layer materials, initial layer thicknesses and fit parameters);

— application of database values for optical or dielectric constants or separate experimental determination of these constants for non-fit parameters;

— applied dispersion formulae.

The condition that the root mean square deviation (D_{RMS}) between measured and simulated curve progressions of Ψ or Δ in accordance with Formula (A.20) will become minimal, will deliver the desired fit parameters, such as layer thickness and refractive index, as the result of an iterative fit procedure (see Figure 3).

NOTE In accordance with ISO/IEC Guide 98-3, the term “error” is no longer used; however, root mean square error (RMSE), instead of D_{RMS}, can be found in many software products.

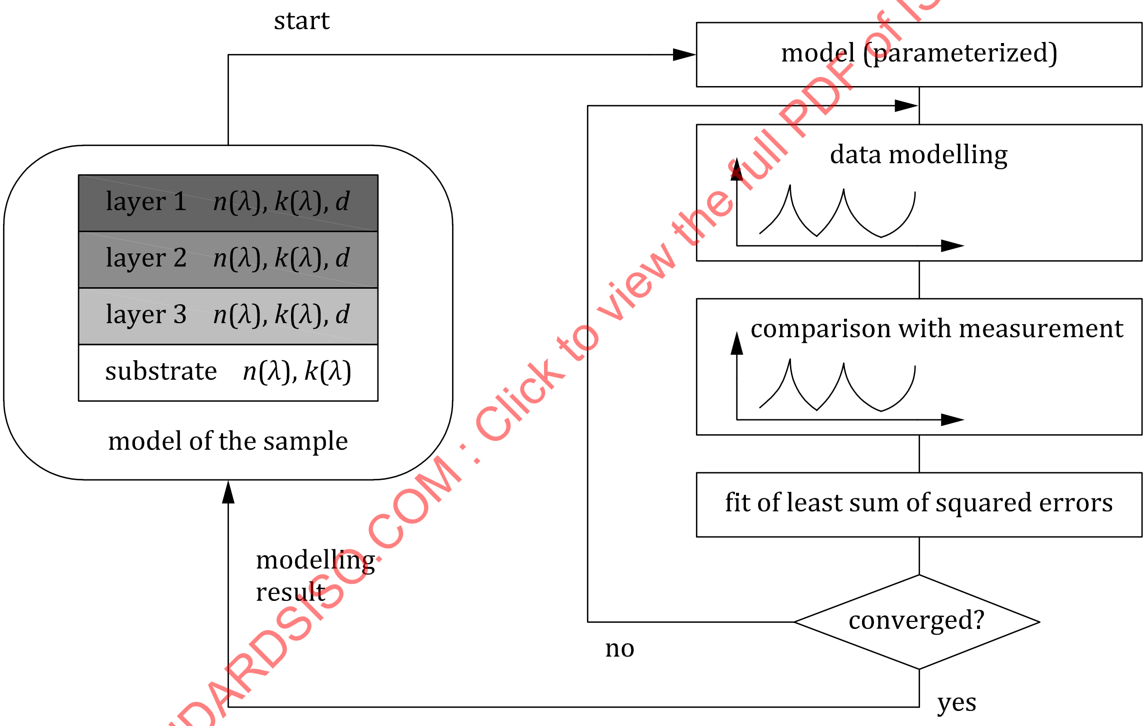


Figure 3 — Schematic representation of the iterative fit procedure

7 Basic models

7.1 General

The ellipsometric transfer quantities Ψ and Δ represent a spectral fingerprint of the surface of the sample and thus can also be used for material identification. When determining optical and dielectric constants/functions as well as layer thicknesses, a model is mandatory. For this purpose, the basic models in accordance with 7.2 to 7.6 are used.

Note Further general information is provided in References [1] to [9].

7.2 Bulk material (case 1 of application)

See DIN 50989-2.

Uncoated, clean, homogeneous and isotropic material of sufficient thickness, so that it is not necessary to consider backside reflections, even for transparent materials.

7.3 Transparent single layer (case 2 of application)

See DIN 50989-3.

Closed layer, for which the light extinction can be neglected.

7.4 Semi-transparent single layer (case 3 of application)

See DIN 50989-4.

Closed layer, for which the light extinction of the layer cannot be neglected.

7.5 Multiple layers and periodic layers (case 4 of application)

See DIN 50989-5.

Layer system consisting of multiple single layers in accordance with 7.3 and/or 7.4 in the form of layer stacks or with several repetitions of two alternating layer materials.

7.6 Effective materials (case 5 of application)

See DIN 50989-6.

Roughness, gradient layers, island layers and composite layers.

8 Raw data

In the past, nulling ellipsometry was developed as the first measuring method in the field of ellipsometry. The ellipsometric transfer quantities Ψ and Δ, which are still widely used today, shall be treated as direct measurement data exclusively within in the framework of nulling ellipsometry. For many devices (RAE, RCE, RPE, etc.), these parameters are currently generated from the modulated intensity signal using Fourier analysis. However, in the meantime, a further method has been established, which bypasses the Fourier analysis originating from analogue signal processing and instead directly calculates Ψ and Δ values per fit from measurement data. Thus, each time errors are being analysed, it shall be observed that in many cases even the ellipsometric transfer quantities (in terms of raw data) often represent the result of a fit process.

For these reasons, the approach to raw data processing has been shifted from the parameters Ψ and Δ to quantities that are more beneficial to modern metrology. Examples are calculating with Stokes vectors and calculating with elements of the Jones or Mueller matrix. Currently, calculating with the single elements N_M, C_M and S_M of the Mueller matrix [see Formula (A.23)] is considered the most suitable method to ensure a stringent uncertainty analysis, see Annex A.

9 Verification of correct adjustment of the device

9.1 Straight line measurement

By means of the straight-line measurement, it is verified that measuring the polarization state is conducted correctly by the ellipsometer. This measurement is widely unaffected by the geometric adjustment of the goniometer for determining the angle of incidence. Should severe adjustment errors occur in the goniometer, then this measurement mostly fails due to an insufficient signal.

For a measurement without reflection at straight beam guidance from the light source to the receiver module, in the absence of objects in the optical path, the measurement ideally delivers the following results: $\Delta = 0°$ and $\Psi = 45°$ at each wavelength.

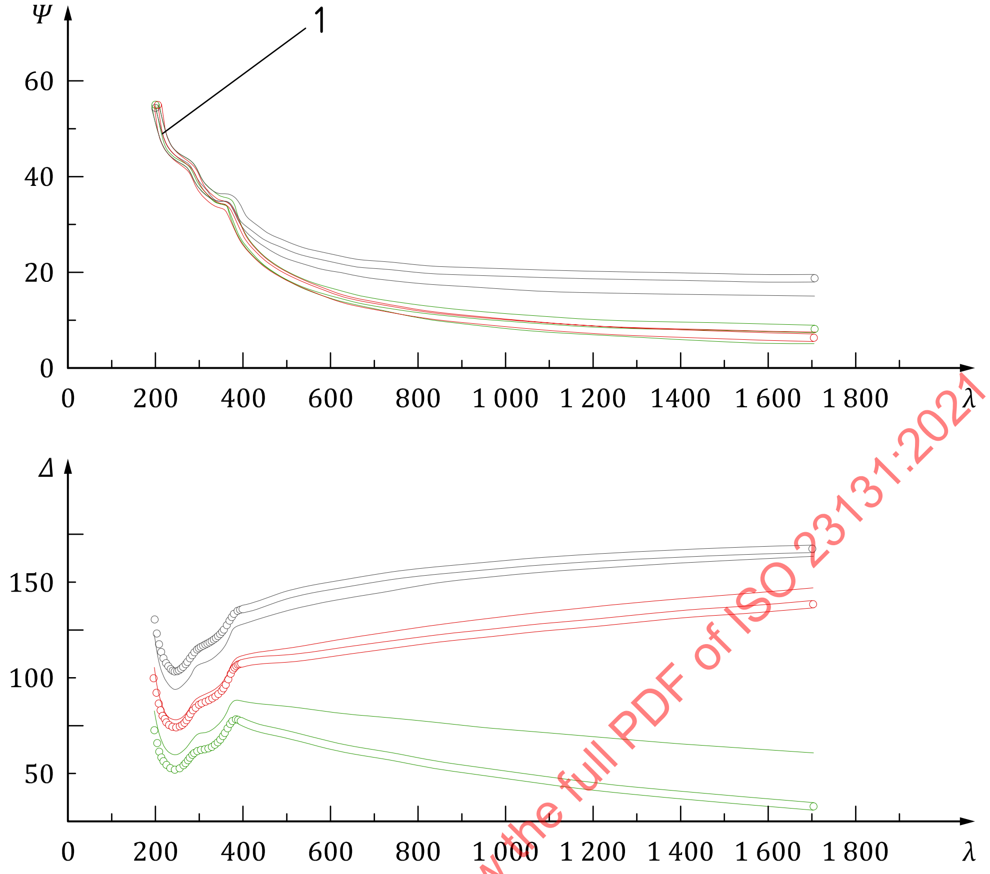
For an isotropic Mueller matrix measurement, for which only the parameters N_M (= $-M_{21} = -M_{12}$), C_M (= $M_{33} = M_{44}$) and S_M (= $M_{34} = -M_{43}$) are considered, the measurement ideally delivers $N_M = S_M = 0$ and $C_M = 1$ (4 × 4 identity matrix).

For REE (rotating element ellipsometer) devices, the deviations for Ψ should be less than ±0,1° and for Δ less than ±1°.

9.2 Simple measurement of angles

9.2.1 Measurement on a known sample, e.g. SiO_2/Si, with fitting of the angle of incidence

An analysis including various angles of incidence can be used to verify the correct adjustment of the angle of incidence. This method is illustrated in Figures 4 and 5. If the actual angles of incidence do not correspond to the nominal angles of incidence, this can be determined by appropriate measurement and analysis. However, a prerequisite is that a robust model is already available for this analysis, including optical constants, which do not need to be determined first. Otherwise, there is the risk that the number of degrees of freedom is too high, which leads to the fact that the correct functioning of the fit is spuriously pretended. For example, a calibration sample, which has already been characterized by a correctly adjusted device and for which consequently correct data records for the optical constants of all materials and the layer thickness are available, is appropriate for this purpose. When comparing a measurement on the reference material at incorrectly adjusted or determined angles of incidence of 62°, 71° and 77° with a measurement at the correct angles of incidence of 65°, 70° and 75°, a clear discrepancy is observed (see Figure 4).

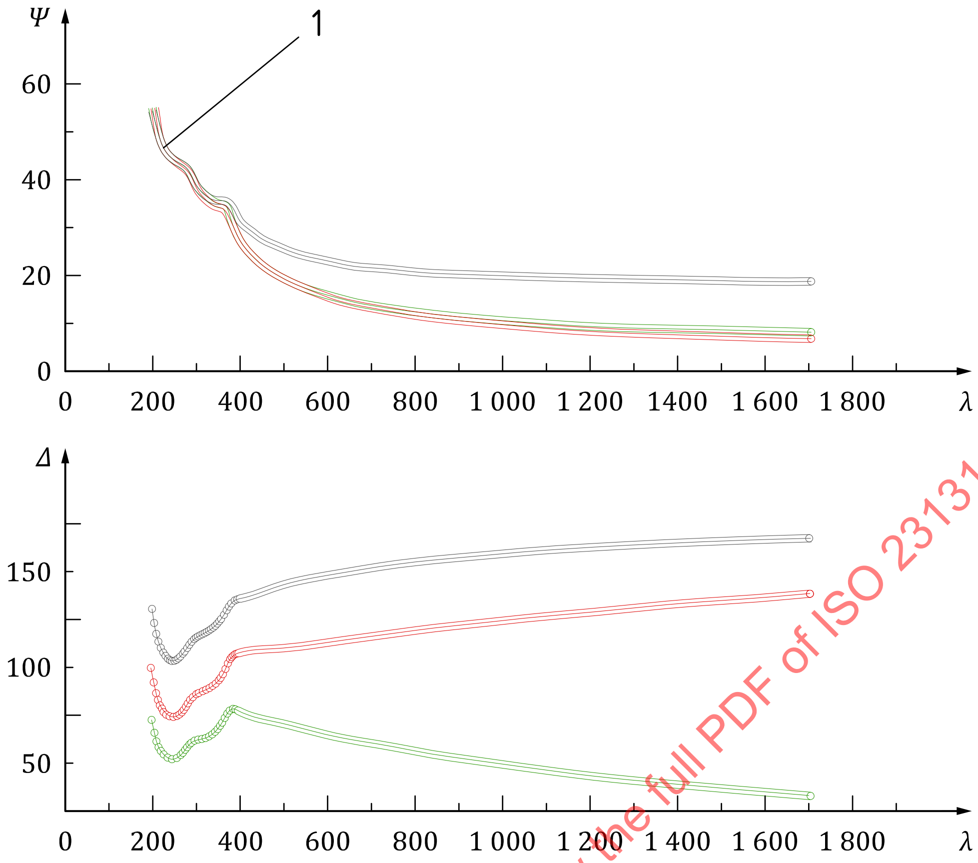


Key

λ	nm	———	75°	○	77°
Δ	degree	———	70°	○	71°
Ψ	degree	———	65°	○	62°
1	25 nm SiO_2 on Si				

Figure 4 — Measurement on a known reference material and at incorrectly adjusted angles of incidence

The analysis of the data record for an incorrect adjustment shows that no curve fitting with a satisfying D_{RMS} will be achieved at incorrectly adjusted (i.e. incorrectly determined) angles of incidence. The agreement of the curves in Figure 4 is notably unsatisfying and hence the result is incorrect. This represents a mechanism of self-control, which is inherent to ellipsometry. However, this self-control only works if there is no fundamental doubt about the model to be used (e.g. SiO_2 on Si) and if this model is not solely designed at a greater level of complexity for the purpose to simply achieve good agreement. If the fit applied on the angle of incidence is also allowed, the incorrectly adjusted angles of incidence of 62°, 71° and 77° as well as the layer thickness will be determined correctly and the agreement of both curve pairs is perfect (see Figure 5).



Key

λ	nm	(grey line)	77°	○ (grey)	77°
Δ	degree	(red line)	71°	○ (red)	71°
Ψ	degree	(green line)	62°	○ (green)	62°
1	25 nm SiO_2 on Si				

Figure 5 — Fit applied on the (incorrectly adjusted) angles of incidence for the measurement in accordance with Figure 4

9.2.2 Measurement of the Brewster's angle of water, of a solvent or of technical glass

This measurement serves as a simple and high-precision test for the correct adjustment of the angle of incidence φ of the goniometer of ellipsometers. The measurement of high-purity water is considered to be the type of measurement with the highest precision. Rotating ellipsometer components can emit strong vibrations so that no calm water surface can be established. An alternative in such cases is, for example, the surface of a technical glass. For both options, capturing backside reflections shall be absolutely eliminated, e.g. by means of sufficiently thick bulk material, surface wrinkling of the backside, non-reflecting surfaces in water.

Sources of error for this method are:

— water: movement of the water surface due to mechanical shocks, impact sound, vibration of devices due to rotating elements, vacuum pumps, etc.;

— water: contamination of water, especially due to floating substances, such as oils and fats forming a film on the surface;

— glasses: assuming bulk material can be wrong, e.g. due to finishing artefacts or glass degradation on the surface, due to roughness, surface layers or adsorbates;

— general instrument-related sources of error for ellipsometers, such as collimation error (leading to uncertainty regarding the angle of incidence) and the resolution of the monochromator (leading to uncertainty regarding the wavelength); these shall also be considered for this measurement.

10 Verification of the device regarding correct calibration

For this purpose, well-defined clean, homogeneous and isotropic surfaces of bulk material and layer thickness standards can be used as reference materials after successful device adjustment.

11 Test report

The test report shall include at least the following information:

a) a reference to this document, i.e. ISO 23131:2021;

b) a declaration of the model used and of all relevant sample-related, measurement-related, model-related and simulation-related parameters in accordance with Clauses 5, 6 and 7;

c) a presentation of the fit result with uncertainty in accordance with ISO/IEC Guide 98-3;

d) the date and name of the test inspector.

Annex A
(informative)

Mathematical and physical principles of ellipsometry

A.1 Optical parameters

The optical parameters are:

— wavelength λ [index a (for ambient) relating to the environment; index s relating to the substrate, index 1 relating to the topmost layer adjacent to the environment, successively counting to the lowermost layer with the largest index bordered by the substrate];

— speed of light c;

— speed of light inside the medium c (with the appropriate index);

— the relationship between frequency ν and circular frequency ω, as represented in Formula (A.1).

$$\omega=2\pi\nu \quad \text{(A.1)}$$

— the relationship between wavelength c and frequency ν, as represented in Formula (A.2).

$$c=\lambda\nu \quad \text{(A.2)}$$

A.2 Optical material constants and function

The complex refractive index N can be determined with Formula (A.3).

$$N=n(\lambda)+i\times k(\lambda) \quad \text{(A.3)}$$

where

n is the refractive index, the real part of the complex refractive index at a given wavelength;

k is the extinction coefficient, the imaginary part of the complex refractive index at a given wavelength.

The optical function shows the dependence of the optical constants $n(\lambda)$ and $k(\lambda)$ on wavelength.

A.3 Dielectric constants and function

The (complex) dielectric function can be determined with Formula (A.4).

$$\varepsilon=\varepsilon_1(\omega)+i\times\varepsilon_2(\omega) \quad \text{(A.4)}$$

where

ε_1 is the real part of the dielectric function at a given circular frequency ω;

ε_2 is the imaginary part of the dielectric function at a given circular frequency ω.

The dielectric function shows the dependence of the dielectric constants $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ on frequency.

The dispersion shows the dependence of the optical or dielectric function on wavelength or frequency, respectively.

A.4 Relationship between complex refractive index N and dielectric function ε

The relationship between the complex refractive index N and the dielectric function ε is represented in Formulae (A.5) and (A.6).

Formulae (A.7) and (A.8) show the relationship of optical and dielectric constants.

$$\varepsilon = N^2 \tag{A.5}$$

$$\varepsilon = (n + i \times k)^2 = n^2 - k^2 + 2 \times i \times n \times k = \varepsilon_1 + i \times \varepsilon_2 \tag{A.6}$$

resulting in

$$\varepsilon_1 = n^2 - k^2 \tag{A.7}$$

and

$$\varepsilon_2 = 2nk \tag{A.8}$$

A.5 Definition of the pseudo-dielectric function

The pseudo constants or pseudo functions N and ε are the results of the ellipsometric transfer quantities assuming that the measured system is a homogeneous and isotropic bulk material. In contrast to the optical/dielectric material constants/material functions, which are independent of the angle of incidence in the case of homogeneous and isotropic materials, the pseudo constants/functions result in a dependence on the angle of incidence if and only if the assumed model including bulk material is not applicable, such as in presence of a transparent coating. This ellipsometric case is the only case that can be described analytically, as described in Formula (A.9).

$$\langle \varepsilon \rangle = \sin^2 \varphi \left[1 + \tan^2 \varphi \left(\frac{1-\rho}{1+\rho} \right)^2 \right] \tag{A.9}$$

A.6 Interface parameters

The amplitude reflection coefficient of p- or s-polarized, reflected r to incident i light can be described in accordance with Formula (A.10) or (A.11).

$$r_\mathrm{p} = |r_\mathrm{p}| e^{\mathrm{i}\delta\mathrm{p}} = E_\mathrm{rp} / E_\mathrm{ip} \tag{A.10}$$

$$r_\mathrm{s} = |r_\mathrm{s}| e^{\mathrm{i}\delta\mathrm{s}} = E_\mathrm{rs} / E_\mathrm{is} \tag{A.11}$$

where E is the electric field strength.

