INTERNATIONAL STANDARD

ISO 23131

First edition
2021-04

Ellipsometry — Principles

Ellipsométrie — Principes

Reference number
ISO 23131:2021(E)

ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Email: copyright@iso.org
Website: www.iso.org

Published in Switzerland

Contents

Page

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).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

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

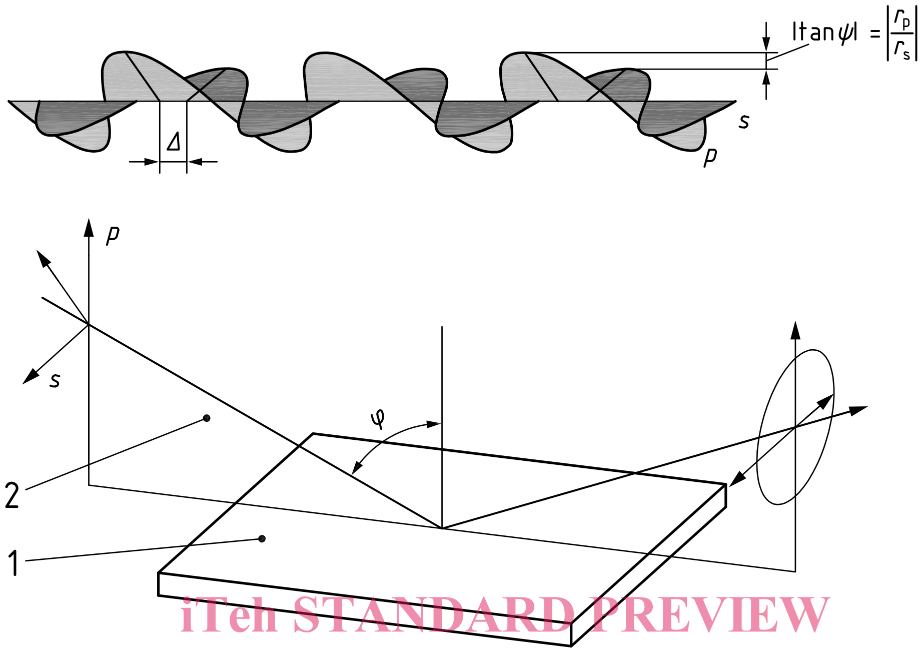
— IEC Electropedia: available at http://www.electropedia.org/

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).



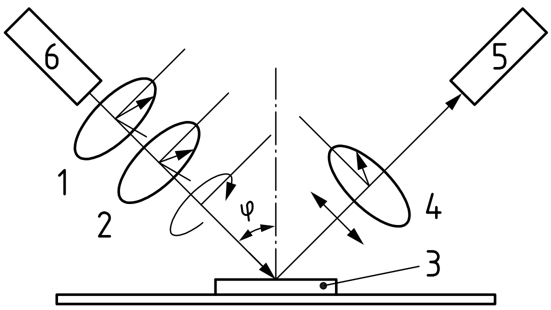
Key

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.

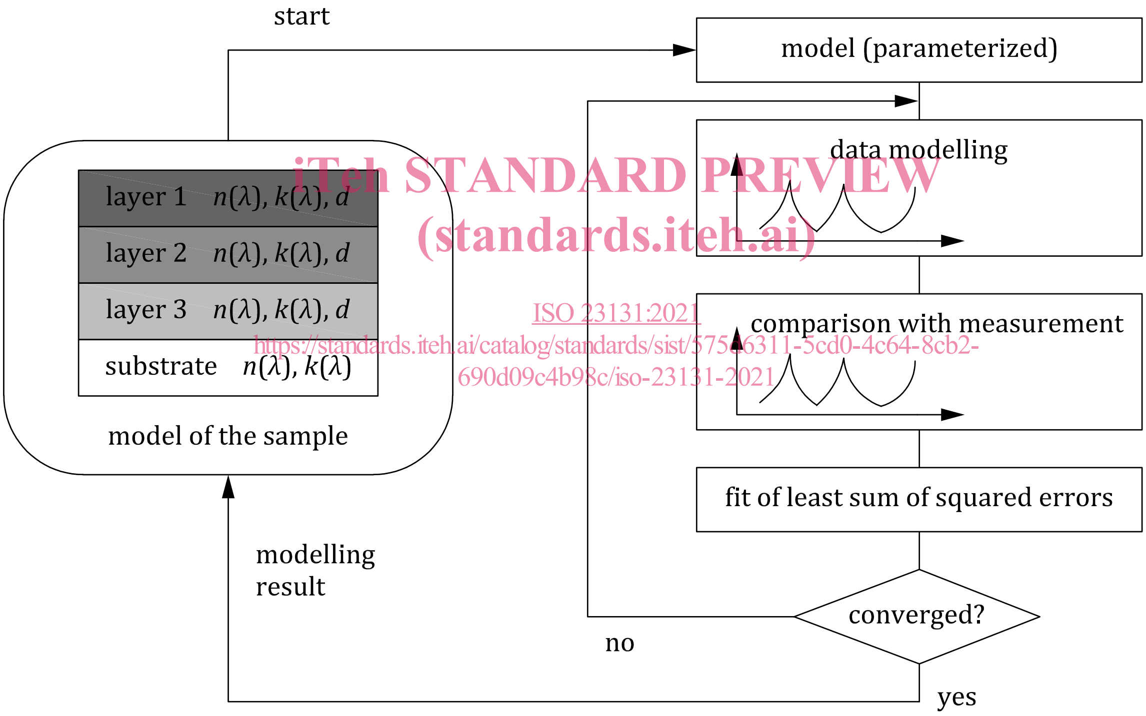


Figure 3 — Schematic representation of the iterative fit procedure

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