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Introduction

This draft standard is based on national and international discussions. Your comments on this draft are invited and will assist in the preparation of the consequent standard.

For international standards, comments will be reviewed by the relevant UK national committee before sending the consensus UK vote and comments to the international committee, which will then decide appropriate action. If the international standard is approved, it is usual for the text to be published as a British Standard.

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Submission of Comments

- **Annotated drafts are not acceptable and will be rejected.**
- All comments should be submitted online at <https://standardsdevelopment.bsigroup.com/>. You will need to register in order to comment.

Template for comments and secretariat observations

Date: xx/xx/20xx	Document: ISO/DIS xxxx
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1	2	(3)	4	5	(6)	7
MB	Clause No./ Subclause No./Annex (e.g. 3.1)	Paragraph/ Figure/Table/Note	Type of comment	Comment (justification for change) by the MB	Proposed change by the MB	Secretariat observations on each comment submitted
	3.1	Definition 1	ed	Definition is ambiguous and needs clarifying.	Amend to read '...so that the mains connector to which no connection...'	
	6.4	Paragraph 2	te	The use of the UV photometer as an alternative cannot be supported as serious problems have been encountered in its use in the UK.	Delete reference to UV photometer.	



DRAFT International Standard

ISO/DIS 23131-3

Ellipsometry — Part 3: Transparent single layer model

ICS: 17.020

ISO/TC 107

Secretariat: **KATS**

Voting begins on:
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Voting terminates on:
2025-04-01

Member bodies are requested to consult relevant national interests in ISO/TC 35/SC 9 before casting their ballot to the e-Balloting application.

This document is circulated as received from the committee secretariat.

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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/JWG 4 "Joint ISO/TC 107 – ISO/TC 35/SC 9 WG: Thickness measurement methods for coatings, paints and varnishes".

A list of all parts in the ISO 23131 series can be found on the ISO website.

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 in the field of integrated production — originally 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 transfer quantities Ψ (Psi, amplitude information) and Δ (Delta, phase information), based on which the physical target quantities 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 detect 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.

In the *transparent single layer* model, a fitting procedure is used to determine the layer thickness d and the refractive index n of the layer while the optical constants of the substrate are known. For ideal transparent materials, it is assumed that $k = 0$. Therefore, fitting only refers to the layer thickness d , which is by definition independent of the wavelength and of the angle of incidence, and the wavelength-dependent refractive index n , which does not depend on the angle of incidence. Consequently, the *transparent single layer* model allows the determination of the layer thickness and of the refractive index.

Ellipsometry —

Part 3: Transparent single layer model

1 Scope

This document uses ellipsometric measurements and their analysis to specify the method for the determination of the layer thickness d of a transparent layer and the optical (refractive index n) or dielectric (real part ε_1) constants/functions based on the *transparent single layer* model within a spectral region, for which $k = 0$ applies.

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 23131, *Ellipsometry — Principles*

ISO/DIS 23131-2:2024, *Ellipsometry — Part 2: Bulk material model*

ISO/IEC 17025, *General requirements for the competence of testing and calibration laboratories*

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

3 Terms and definitions, symbols and abbreviations

3.1 Terms and definitions

For the purposes of this document, the following term and definition apply.

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

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <https://www.electropedia.org/>

3.1.1

transparent single layer

layer of which the light extinction can be neglected within the considered spectral region.

3.2 Symbols and abbreviations

[Table 1](#) shows all the symbols and abbreviations used throughout this document in addition to those of ISO 23131 and ISO/DIS 23131-2:2024, taking into account the requirements of ISO/IEC Guide 98-3 and ISO/IEC 17025.

Table 1 — Symbols and abbreviations

Symbols and abbreviations	Description
n	refractive index (real part of the complex refractive index N)
k	extinction coefficient (imaginary part of the complex refractive index N)
N	complex refractive index
ε_1	real part of the complex dielectric function
ε_2	imaginary part of the complex dielectric function
ε	complex dielectric function
φ	angle of incidence between the incident light wave and the normal to the surface
N_a	complex refractive index of the ambient space
N_l	complex refractive index of the layer
N_s	complex refractive index of the substrate
R_t	maximum roughness depth
R_a	arithmetic roughness average (profile roughness)
D_{RMS}	root-mean-square deviation (in ISO 23131 and some evaluation software, <i>RMSE</i> (root-mean-square error) is still used)
$D_{\text{RMS,min}}$	minimum of the root-mean-square deviation
d_{fit}	fitting result for the layer thickness of the transparent single layer (sample)
d_{calc}	calculated layer thickness of the transparent single layer for single-wavelength ellipsometry and a single angle of incidence (sample)
u_{fit}	uncertainty of the fit on the layer thickness model parameter (sample)
a	half width of the rectangular distribution
u_{mod}	uncertainty of modelling in the <i>transparent single layer</i> model regarding the layer thickness (sample)
$u_{\text{fit,ref}}$	uncertainty of the fit on the layer thickness model parameter (layer thickness standard/reference layer)
U_{ref}	expanded combined uncertainty (measurement uncertainty) of the reference materials (layer thickness standard/reference layer)
c_{ref}	coverage factor ^a that has been used to indicate the measurement uncertainty (expanded combined uncertainty) of the reference materials (layer thickness standard/reference layer)
u_{ref}	combined uncertainty of the layer thickness (layer thickness standard/reference layer)
u_d	combined uncertainty of the layer thickness d considering all uncertainty components (sample)
c_{samp}	coverage factor ^a for expression of measurement uncertainty (expanded combined uncertainty) of sample

^a The coverage factor is denoted “ k ” in ISO/IEC Guide 98-3.

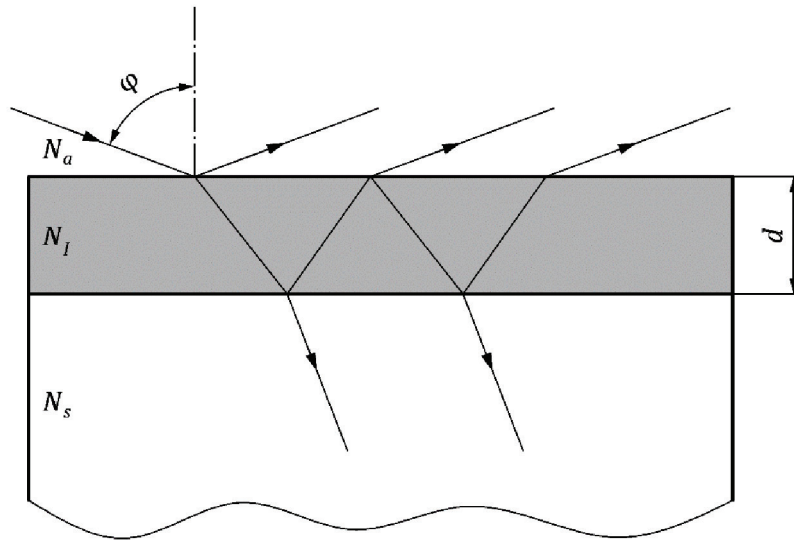
4 Transparent single layer model

4.1 Optical path

[Figure 1](#) shows the optical path at a certain angle of incidence φ in the *transparent single layer* model. The ambient space (index “ a ”) will be assigned with the complex refractive index N_a . Usually, air will serve as the ambient space and the refractive index will actually be in close approximation with $n_a = 1,000$ and $k_a = 0,000$. The transparent single layer will be assigned with the layer thickness d and the complex refractive index N_l (index “ l ” for layer). In the *transparent single layer* model, it is assumed that $k_l = 0$. The substrate will be assigned with the complex refractive index N_s .

Incident light from the ambient space will strike the interface between the ambient space and the transparent single layer; part of it will be reflected. Another part will be refracted and experiences multiple reflections

in the transparent single layer at the layer/substrate and the layer/ambient interfaces. The measured signal thus represents the superposition of the multiple reflections (interference) in the transparent single layer.



Key

- φ angle of incidence between the incident light wave and the normal to the surface
- N_a complex refractive index of the ambient space (for air real, $N_a = n_a = 1,000$)
- d layer thickness of the transparent single layer
- N_l complex refractive index of the layer (for transparent layers real, $N_l = n_l(\lambda)$, $k_l(\lambda) = 0$)
- N_s complex refractive index of the substrate ($N_s = n_s(\lambda) + i \cdot k_s(\lambda)$)

Figure 1 — Optical path in the *transparent single layer* model

In the *transparent single layer* model it is assumed that in addition to the angle of incidence φ only the layer thickness d and the refractive index n_l or the real part of the dielectric function ϵ_{1l} of the layer as well as the optical (n_s , k_s) or dielectric (ϵ_{1s} , ϵ_{2s}) constants of the substrate will determine the measured ellipsometric transfer quantities Ψ and Δ .

Annex A.1 gives the refractive indices of specified transparent layer materials. Annexes A.2 and A.3 describe the reference layers for transparent single layers on opaque or transparent substrates.

4.2 Assumptions

4.2.1 General

The following model assumptions given in Table 2 will be made for the *transparent single layer* model.

Table 2 — Assumptions for the *transparent single layer* model

Assumption	Description
M1	negligible extinction (i.e. neither absorption nor scattering losses) of the layer ($k_1(\lambda) = 0$) in the considered spectral region
M2	no layers in addition to the transparent single layer, neither on the single layer (e.g. moisture or dirt films) nor between the layer and the substrate (e.g. interfacial layers)
M3	negligible roughness of the layer (and of the substrate) relative to the measurement wavelength λ : typically, R_a or $S_a \leq \lambda/250$ negligible maximum roughness depth relative to the layer thickness d : typically $R_t \leq 1 \text{ nm} + d/1\,000$
M4	homogeneity of the substrate and the layer, especially of the layer thickness d in the field of analysis (FOA), i.e. no lateral (x - y) or vertical (z) local dependence (gradients) of the optical or dielectric constants
M5	isotropy or known anisotropy of the layer (and of the substrate), i.e. no unknown directional dependence of the optical or dielectric constants
M6	defined chemical composition, crystallographic microstructure and atomic packing factor of the layer (and of the substrate) with sufficient stability (relative to the measuring time)
M7	only the layer surface and the layer/substrate interface but not the backside reflections of transparent substrates will contribute to the reflected signal, i.e. the use of substrates of sufficient thickness, typically of more than 5 mm
S1	planarity of the sample's surface in relation to the orientation of the beam path during the measurement, i.e. conformity of the layer's surface with the ellipsometer reference plane to obtain a symmetric optical path
S2	consistency between the angle of incidence φ applied during measurement and the one used in the model

Assumptions M1 to M7 specify the influencing parameters related to the layer and substrate material and assumptions S1 and S2 describe measurement-related influencing parameters which are relevant for the validity and quality of the *transparent single layer* model.

The transparent reference layers described in annex A.2 comply with model assumptions M1 to M7 in very close approximation. When measuring actual materials and surfaces, several assumptions of the *transparent single layer* model may not be met. The fundamental model-specific requirement is assumption M1. Possible deviations from the assumptions M2 to M7 and S1 to S2 are specified for the *bulk material* model in ISO/DIS 23131-2:2024 and shall apply accordingly to the *transparent single layer* model in this document.

4.2.2 Deviations from model assumption M1

Absorption or scattering losses occurring in the considered spectral region will cause non-conformance with assumption M1. It shall be noted that it is nearly impossible to capture extinction coefficients $k_1(\lambda) \leq 0,1$ by using ellipsometry as a method which measures in reflection.

4.2.3 Deviations from model assumption M2

As a result of the manufacturing process of the transparent single layer, interfacial layers can develop, which then also need to be taken into account in the model.

4.2.4 Deviations from model assumption M3

Physical substrate surfaces show some type of roughness that will cause losses due to scattering as well as depolarization effects. If model assumption M3 is not met, the roughness can be described as the interfacial layer between the substrate and the transparent single layer (as well as between the transparent single layer and the ambient space in case of roughness of the layer surface) using the effective medium theory.^[1] The maximum roughness depth R_t , which is a multiple of the arithmetic mean roughness value R_a , is usually applied as the thickness of this interfacial roughness layer (see Figure 2).