Spectroscopic Ellipsometry Set-ups for Spectral Determination of Optical and Dielectric Material Properties and Layer Thicknesses

Key words

Spectroscopic ellipsometry, reflection, polarisation, refractive index n, extinction coefficient k, layer thickness h, dielectric function (real and imaginary parts ε_1 and ε_2), energy loss function

Fields of application

Development and certification of reference materials and layers; reference procedure for the determination of optical material constants and their dispersion and thicknesses from the lower nanometer to the micrometer range. Homogeneity, stability and identification testing of surfaces and thin films.

Methodology and instrumentation

Methodology: Reflection experiment with polarised light. Instrumentation:

1. Gonio-spectroscopic ellipsometer VASE / WOOLLAM (monochromator, autoretarder, AOI automatically adjustable)
2. Gonio-spectroscopic ellipsometer M2000DI / WOOLLAM (polychromatic detection, RCE, AOI automatic adjustable, mapping-table
3. Single wavelength laser ellipsometer SE 400 / Sentech (HeNe-Laser, AOI manually adjustable),
4. VUV ellipsometer at synchrotron beamline BESSY-II (cooperation with TU Berlin and ISAS AOI manually adjustable, energy range 2.4 eV – 35 eV)
5. FTIR ellipsometer Sendira / Sentech, (FTIR-spectrometer 400 cm-1 – 6000 cm-1, AOI automatically adjustable)
6. Imaging-nulling-ellipsometer EP3-SE / Accurion (AOI automatically adjustable,
   spectral range 350 nm – 1000 nm, best lateral resolution depending on sample: 2 µm – 5 µm)

Items tested

Bare and coated surfaces which allow from their properties (roughness, isotropy, homogeneity) the investigation by ellipsometry. Complex dielectric multi-layers. Metals, semiconductors and polymers.

Quantities / characteristics tested

Ellipsometric quantities tan Ψ and cos Δ (amplitude and phase information) of bare and coated ($1 \text{ nm} < h < 10$ µm) samples in the wavelength range $100 \text{ nm} < \lambda < 1.7$ µm. A parametric fit procedure determines optical (n, k) or dielectric (ε1, ε2) material quantities and layer thicknesses for at least semi-transparent films.

Uncertainty / reliability of results

Optical / dielectric constants (n, k, ε1, ε2): 0.01 – 0.05; thickness h: 0.5 nm – 10 % h relative uncertainty

Qualification and quality assurance

Inherent traceability of calibration, application of certified standards and reference materials (NIST, PTB, BAM, VLSI); participation in international inter-laboratory comparisons; spectroscopic ellipsometry in the given wavelength range (VUV-UV-vis-NIR) because of the variety of methods (RAE, RPE, SE, SWE) and material data bases unique in Germany. Development of standards (PAS 1022) leading in the world.

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Further information

Principle of operation

Ellipsometry is a reflection experiment with polarised light whereby the change of the polarisation state upon reflection is measured both for parallel and perpendicular components of light. This enables the determination of amplitude and phase information (Ψ and Δ). A parameterised model for the layer-substrate system is optimised by fitting the theoretical values of Ψ and Δ on the experimental data of the ellipsometric quantities Ψ and Δ by a least squares method. This procedure yields in a set of physical quantities (n and k or ε_1 and ε_2) dependent on the wavelength. Additionally, film thicknesses h independent of the wavelength can be derived. Measurements at different angles of incidence (AOI) are used for the validation of the model or to improve the quality of the fit. Without any modelling and data fitting, ellipsometric quantities tan Ψ and cos Δ represent a fingerprint spectrum of the investigated material, i.e. of the electronic structure as well as of the layer thicknesses. This is of great importance for the identification, homogeneity and stability testing of layer-substrate systems.

Equipment

Fig. 1: left: UV/vis/NIR gonio-spectral ellipsometer Woollam VASE
right: VUV spectral ellipsometer at beamline BESSY II (co-operation with TU Berlin and ISAS Berlin)

Fig. 2: left: Single wavelength ellipsometer (Sentech SE400)
right: UV-vis-NIR spectral ellipsometer (Woollam M2000DI)

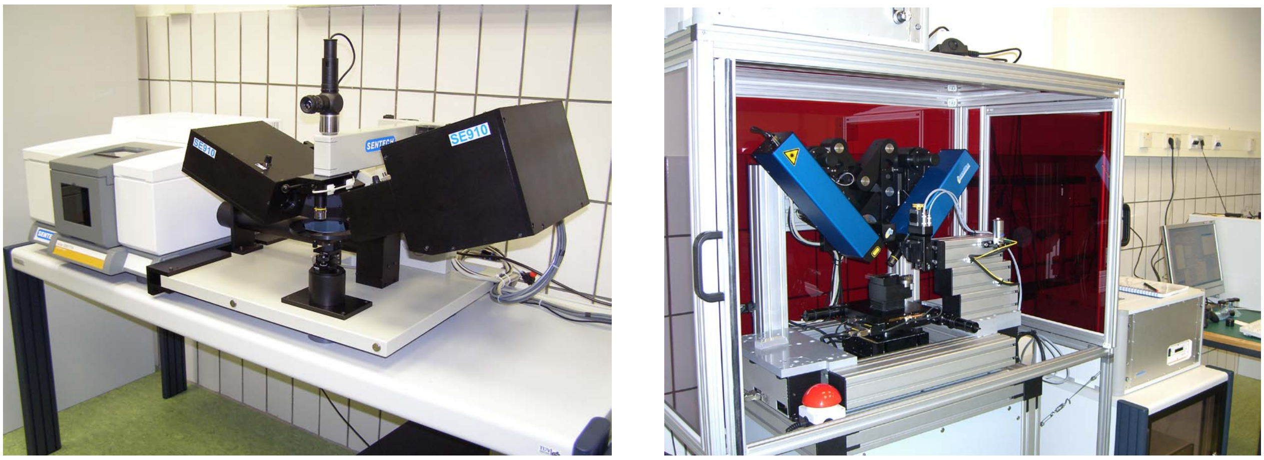

Fig. 3: left: FTIR-ellipsometer (Sentech SENDIRA)
right: Imaging ellipsometer (Accurion EP^3-SE)

The equipment employed includes several ellipsometers which can be chosen according to the measurement task (Figs. 1 – 3). In the visible range, mainly the spectroscopic ellipsometers VASE und ESG4 are applied. For faster measurements (e. g. the analysis of homogeneity) the laser ellipsometer SE400 is the system of choice. Measurements in the deep UV region are carried out at the BESSY II.

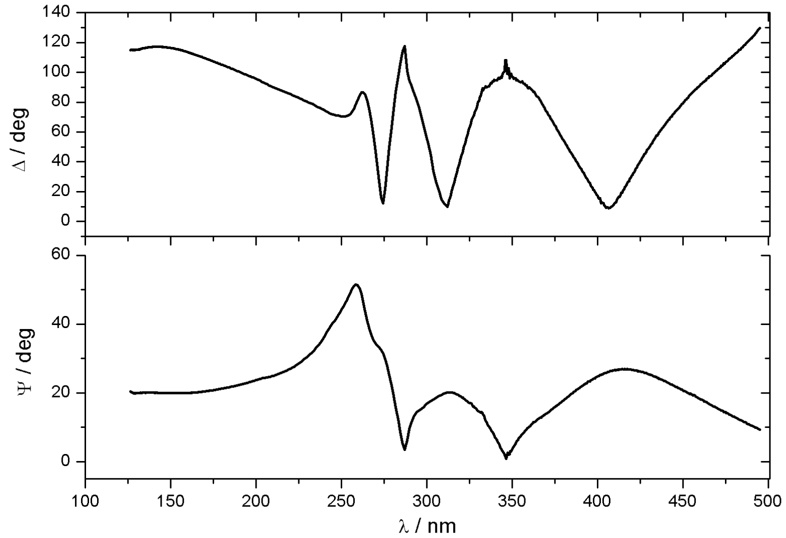

Fig. 4: Ellipsometric measurement in the VUV-range for Ta_2O_5 on silicon

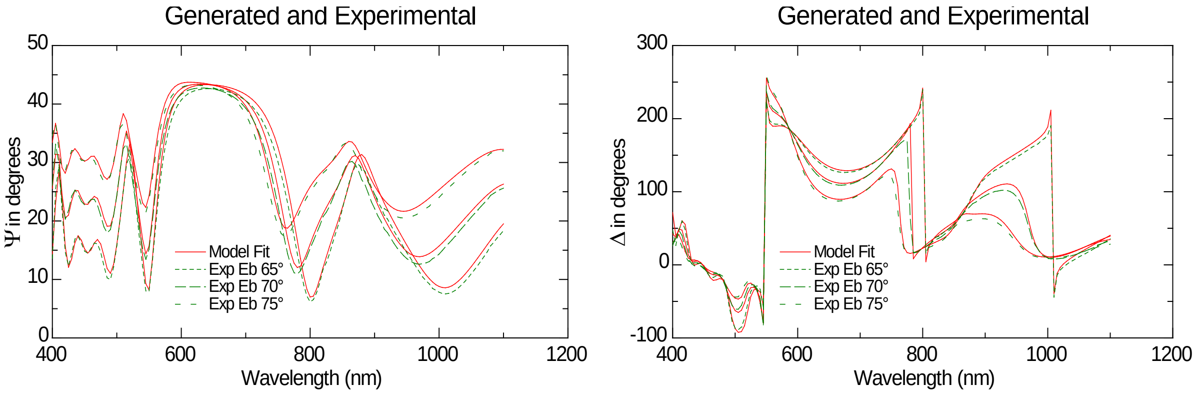

Fig. 5: Ellipsometric analysis of a 10-layered system (reference material BAM-L101)

Examples

Figs. 4 and 5 show examples of measurements with the equipment described above. VUV ellipsometry allows the determination of the band structure down to very short wavelengths. Measurements in the visible range are best for analysing dielectric layer systems. Such a layer system is provided by BAM and certified by means of spectroscopic ellipsometry (BAM-L101, see Fig. 5). In this case, ellipsometry was used for the determination of the total layer thickness of the stack.

Requirements for samples investigated

Flat surfaces of small roughness (typically $< \lambda/10$) consisting of a single phase material or material mixtures of two effective-media-materials (including voids) can be analysed. Surface of inspection and reverse side should be sufficiently parallel. For the investigation of layer-substrate systems, the availability of bare as well as coated substrates may be very helpful. The independent determination of the optical constants of an unknown film material inside a multilayer stack from a single layer (of sufficient thickness) on a reference material may be required for gaining uncertainties claimed before.

Accuracy of the measurement

The wavelength scale is calibrated with several spectral lines as internal standard with an accuracy of about ± 0.1 nm. The calibration of the set-up itself is standard-free. For the validation of the calibration of the $\tan\Psi$ and $\cos\Delta$ -scales certified reference materials are employed. The accuracy of $\tan\Psi$ und $\cos\Delta$ is then determined mainly by the properties of the sample to be investigated.

Uncertainty of the results

The uncertainty is determined by the properties of the experimental set-up as well as by the properties of the sample to be investigated. Surface roughness has a big influence on the uncertainty. The lower thresholds mentioned above are only valid for an ideal sample and spectral measurement.