accurion
solutions for science

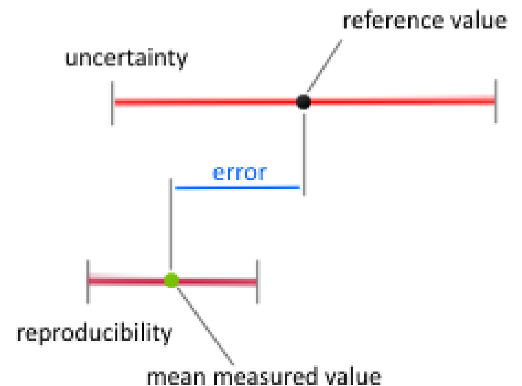
COMPENDIUM

Imaging ellipsometry - Ellipsometric Accuracy of the nanofilm_ep3 series

DIRK HÖNIG

ACCURACY, PRECISION, REPEATABILITY & REPRODUCIBILITY

The comparison and qualification of different instruments is complicated due to inconsistent terms and definitions. We try to adhere to the standards defined in the GUM (*Guide to the expression of uncertainty in measurement*, edition JCGM 100:2008) which is internationally accepted.



The term *accuracy* should be used only as a qualitative expression, as it may not be expressed numerically. The reason is that the "true value" of a measurand is unknowable. Especially in the case of thin films this is quite obvious: the measurand "film thickness" may not be assigned a single true value, as the layers do not have ideally sharp boundaries. Depending on the physical principle of measurement, the boundaries may be located elsewhere and somewhat arbitrarily (imagine for comparison the tip of an AFM, sensing short distance atomic forces while the ellipsometer senses the transition of the refractive index from the layer to the ambient medium).

So even if the measurement has a high repeatability (see below) and all systematic errors are corrected, a true value does not exist and hence no numeric accuracy can be assigned. Therefore, we need to use accepted *reference standards* with specified *uncertainty* to compare our measurements against. The difference between the measurement and the reference is then expressed as the *absolute error of measurement*. Division by the value of the reference then gives the *relative error of measurement*, which is more useful in many practical cases. Our instruments are specified to reproduce the certified values of reference standards within their uncertainty ranges. Hence, our absolute error of measurement spec is equal to the specified uncertainty of the reference (see graphic below).

To specify the *measurement precision*, we use two ways with differing conditions and procedures:
Repeatability is derived by measuring the same sample without changing conditions several times within a short period of time. To avoid drift during the measurement time, thermal equilibrium of instrument, room and sample is presumed. The repeatability is especially important if one wants to measure small differences (e.g. in film thickness) on one sample or to monitor small effects (e.g. adsorption).
Reproducibility is obtained by the following procedure: shut-down of the instrument, removal of the sample, immediate re-start of the instrument, 10min thermal equilibration, re-positioning & alignment of the sample, followed by repetition of the measurement. Ambient temperature is monitored to be stable within +/- 1 K.

From the reproducibility measurement we get a mean measured value $\bar{q}$ and a *standard deviation* $\sigma(q_j) = \sqrt{\frac{\sum_i (q_i - \bar{q})^2}{n-1}}$ of n subsequent measurements q_j. In turn, we can calculate the *error of measurement* for the instrument.

DELTA & PSI, RESOLUTION AND SENSITIVITY

The resolution limit for single measurements in Delta & Psi is the smallest measurable change. This limit is given by the resolution of the angular encoders of the instrument in combination with the null finding algorithm. Because of the systematic nature of this effect, averaging of multiple measurements will not further improve these numbers. The resolution limit is not determined during calibration of each instrument, but confidently given by the design of the instrument. To achieve this resolution in a practical experiment, i.e. to reach a repeatability close to the resolution limit, some conditions must be met. In particular, the resolution depends on the absolute values of Delta & Psi and the experimental conditions. For example, if the light source if the instrument is dimmed, there will not be enough signal swing of the raw signal to determine Delta & Psi accurately, and thus a small change in the samples Delta&Psi will not be observed in the noisy raw signal. But even if the optimal instrument settings are being used, the raw signal might not allow for reaching the limiting resolutions. This is because the raw signal swing is affected by the absolute values of the sample's Delta & Psi, too.

ACCURACY IN FILM THICKNESS OR REFRACTIVE INDEX

The Delta & Psi values translate into a film thickness, refractive index or other physical quantities of interest according to the associated optical (multi-)layer model of the sample under examination. It is obvious that it is more difficult to measure a layer on a substrate of nearly the same material compared to a situation where there is a big difference in the optical properties. For this reason it is not possible to characterize the measurement uncertainties or precision of the instrument by a few numbers. Instead, values are provided for certain reference samples and under well-defined conditions.

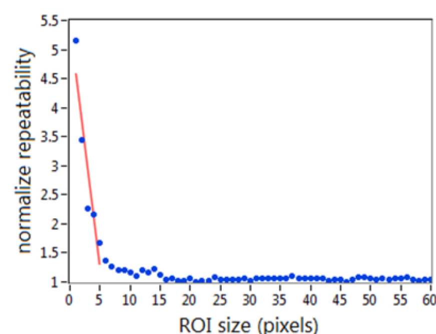
As the Delta & Psi values are periodic with film thickness, it is important to understand that for a particular measurement Delta & Psi may have a different sensitivity, even zero sensitivity. For example, for ultra-thin films <20nm (SiO2/Si), the Psi is essentially insensitive. If one characterizes the ellipsometer only with such a standard, a erroneous calibration in Psi might not be noted. It is therefore important to use at least one reference standard for which Psi is a meaningful measurand.

Consider a repeated measurement of a film changing its thickness in time (e.g. absorption kinetics). The repeatability (see table) defines how the individual results are scattered around a mean value. The mean value has itself a standard deviation of the mean, which is the repeatability devided by the root of the number of measurement. To confidently state a step-like change of the film's thickness, as a rule of thumb the new mean value should differ from the old mean value by at least 3-times the standard deviation of the mean. This sample-dependent number would then define the resolution limit for such a measurement.

PRECISION VS. ROI SIZE

If one compares an imaging ellipsometer (IE) with a conventional ellipsometer, careful consideration of some peculiarities is required. While the conventional ellipsometer feeds the entire light into a single point detector, in an IE the light is distributed over a huge amount of individual sensors, i.e. camera pixels. So each pixel senses only about 10-6 of the incoming total light flux. Here, Poisson

distributed photon noise may become an important factor. This is the case when the available light intensities are low, for example if narrow bandwidth non-laser light sources are being used.



For a direct comparison of ellipsometric instrument quality it might thus be fair to use a rather large ROI averaging over many pixels for the IE. However, to exploit the potential of the IE in terms of spatial resolution, it is important for the user to know how precision is preserved going to smaller ROI sizes.

For very small ROIs or even a single-pixel ROI the photon noise plays the dominant role and SNR will decrease linearly with the size (width, diameter) of the ROI. On the other hand, for larger ROI sizes, pixel averaging does not continue to improve SNR as other effects become dominant. As can be seen from the graph, using a 20x20 pixels ROI will usually perform as good as larger ROIs and is thus a good compromise of ROI size and SNR. Smaller ROIs may benefit from averaging repeated measurements.

Please note that these numbers are provided for orientation only. Several effects may change the ROI size dependency of your actual sample.
Precision vs. measuring time

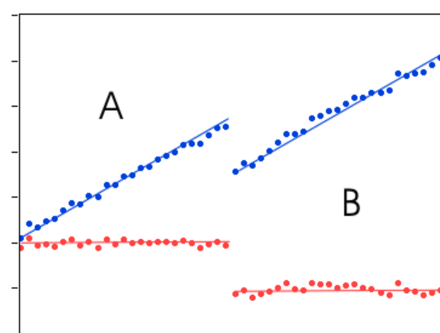
Due to the nature of the null measurement in the EP3, the precision depends on the measuring time: allowing less data points being sampled (script parameter $samples) during the measurement cycle will decrease precision at the benefit of shorter measurement time. This is valid only up to some number of data points from where there will be no further improvement (e.g. due to signal drift). The specs in the table are derived with a number of data points that appears to be optimal by experience.

PRECISION VS. MAGNIFICATION

When switching from the standard nominally 10x objective to the 20x objective, the light from a particular region is spread over a larger area of the CCD camera: the doubled magnification leads to a dilution of the available light per pixel by a factor of 4, causing an increase of photon noise by a factor of 2. On the other hand, the number of pixels averaged into a single ROI also increases by a factor of 4, reducing the noise by the same factor 2. Thus, for a given ROI with a fixed size in microns (not in pixels), the SNR is approximately constant. Note that this considers only the photon noise effects (which are dominant), neglecting camera read-out noise or other artifacts.
It is obvious from the above that when comparing equal ROI sizes in pixels at different magnifications (thus comparing objects of different sizes on the sample) the noise and hence precision will be affected. In the 10x/20x comparison, the 4-times lower light level at 20x will then give rise to doubled noise.

DRIFT

As any instrument also the ellipsometer is exposed to drift, meaning a continuous fluctuation of measured quantities at a time scale larger than the time scale of one individual measurement. The drift in an ellipsometer is generally caused by thermal effects, which makes a temperature controlled environment eligible. Accordingly, precision measurements should be performed only if instrument and sample are in thermal equilibrium and the temperature is maintained stable to approx. +/- 1 K.
Drift is contributing to the overall uncertainty of the measurement and is thus directly coupled to the error of the measurement. It influences in particular the reproducibility, i.e. the repetition of the measurement after waiting for a longer time. In many cases, instrumental drift may be compensated. For example, if a thickness step A→B of a thin film is to be measured, one may measure regions



A and B and compensate for a possible linear drift easily.
The same principle may be applied to kinetic measurements, provided that the drift may be clearly discriminated from the physical effect (e.g. adsorption) being measured.

4-ZONE VS. 1-ZONE NULLING

The nulling procedure applied in the EP3 derives angles of optical components as the basic quantities that are converted into Delta & Psi. If there is a systematic error (a constant bias) in the indication of such an angle, it will be introduced into Delta & Psi and thus contribute to the uncertainty of the measurement. There are some other systematic errors that may play a role. To overcome this, a so-called 4-zone nulling may be applied. Because the errors have different signs for the individual zones they compensate themselves. Besides such angle reading errors various other systematic errors are corrected by 4-zone nulling. Therefore, 4-zone nulling is the method of choice if small error of measurement is required. A detailed description may be found in the book of Azzam . Practically, 4-zone nulling is achieved by measurement of the two conjugated nulls at compensator positions of 45° and -45°, respectively, thus combining 4 measurements into one.

4-zone nulling does not improve the repeatability of the measurement, except for the effect of averaging (which would account for an improvement by a factor of 2, but in practice will not be achieved). Therefore, if only relative effects are to be measured (e.g. a thickness step), 1-zone nulling often does the job with the advantage of shorter measurement times.

MAP HOMOGENEITY

The Imaging Ellipsometer is able to measure 2D maps of ellipsometric parameters. While the ultimate precision may be obtained by measuring always at a reproducible position within the image area, it is also important that there are little image artifacts over the entire field-of-view. This means that for a very homogeneous sample, a Delta or Psi map should ideally appear as a featureless "flat field" according to the specs in the table. This requires strain-free optics and well-collimated, homogeneous illumination.
For the calculation, the standard deviation from the mean along horizontal or vertical profiles is being used.

CALIBRATION

Our standard instruments are calibrated for a wide range of samples and applications, as they occur in a typical case of application in a research lab. As explained before, the uncertainty of measurement is given by comparison with accepted reference standards. However, it is possible to calibrate the instrument to match a specific type of sample. This means that the systematic errors are corrected for a well-defined set of conditions by use of a specific reference sample (or other known information) . For example, if one mainly measures ultra-thin gate oxide layers, it may be convenient to calibrate the instrument to such conditions to reduce the absolute error of measurement. It then would be possible to achieve error levels which are similar to the reproducibility.
If required, it would be possible to calibrate the instrument like this for several applications and switch between them via user selection, scripts or other ways.

REFERENCES

R.M.A.Azzam, M.Bashara (1987) Ellipsometry and Polarized Light, North-Holland, Elsevier, Amsterdam

sample/test	relative error of measurement	absolute error of measurement	precision		comments
			repeatability σ (n=20)	reproducibility σ (n=6)	
0-25nm SiO_2/Si thickness range	9% @ 10nm 3% @ 20nm	0.8nm	0.004nm 0.004° Delta 0.002° Psi	0.02nm 0.02° Delta 0.01° Psi	1-zone n(SiO_2) =1.456 n(Si)=3.83-0.014i
50nm SiO_2/Si	2%	1nm	0.01nm	0.02nm	4-zones n(SiO_2) = 1.456 n(Si) = .83-0.014i
100nm SiO_2/Si	1%	1nm	0.01nm	0.02nm	4-zones n(SiO_2) = 1.456 n(Si) = 3.83-0.014i
Organic film (< 10 nm) on Au	n/a see remarks	n/a see remarks	0.005nm 0.003° Delta 0.004° Psi	0.03nm 0.02° Delta 0.02° Psi	1-zone n(film) = 1.5 n(Au) = 0.164-3.273i
Refractive index of layer, 100nm SiO_2/Si	0.5%	0.01	0.0001	0.0002	derived numerically by conversion of the thickness measurement results, see remarks
Transmission measurement, no sample	*-to be specified-*				AOI=90°, measuring crossed analyzer positions for all combinations P, C=0° or 90°
Spectral characteristics (25nm SiO_2/Si)	maximum deviation of individual wavelength results 0.3nm				(SE models only) 400nm < lambda < 900 nm 4-zones, see remarks
Map homogeneity (25nm SiO_2/Si)	profile standard deviation: Delta 0.1° Psi 0.1°				8x8 pixel binning, laser 658nm or Xe-lamp 590nm
Resolution limits	Delta, Psi, Angle-of-incidence (AOI): < 0.001°				see explanations

- unless otherwise noted, the following conditions apply: standard 10x objective (specifications for other objectives may differ), AOI (angle-of-incidence) 60°, ROI centered w/ size 50x50 pixels , camera gain 50%, laser power 5%, 658nm laser, script parameters $samples=300, $plrange & $alrange adjusted for full camera signal at full polarizer/analyzer swing. Beam profile centered (using z-lift).
- absolute error is based on NIST traceable reference standards from VLSI Inc., see explanations below.
- the 658nm laser is a special wide bandwidth laser source. Other lasers are available, but specs may vary.
- refractive index precision: the same optical model is used as in the thickness measurement, but this time the thickness is kept at the measured value and the data is fitted for a variable refractive index
- organic film on Au: *error of measurement* may not be given due to lacking certified reference samples. As the (potentially anisotropic) organic film refractive index may not be determined independently from the thickness due to general physical limitations for ultra-thin films, usually a reasonable refractive index (e.g. bulk material value) is

assumed and the thickness is determined. Results obtained in this way for densely packed SAM films are consistent with expected values for the respective molecules.

- for the spectral characteristics, the spectrum is fitted for the film thickness, the coefficients of a Cauchy dispersion model for the SiO_2 and the AOI-offset. Then, for each individual wavelength the thickness is checked vs. the spectral result, using the previously determined dispersion and AOI-offset.

All information in this document is subject to modifications. Please check www.accurion.com for the most current revision. The specifications are valid only for instruments manufactured after release of this document.