Uncertainty in measurement of surface topography

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Abstract. With the definition and further standardisation of 2.5-D roughness measuring methods and parameters, the demand of traceability and uncertainty estimation for measurements and parameters automatically becomes eminent. This paper gives an overview of the problems and possibilities that appear when uncertainties have to be put to values that are derived from a measured surface topography such as: the *Ra*-value of a periodic specimen, the *RSm*-value of a type-D standard, the *Sa*-value of a single cut-off length of a type D standard. It is shown that straightforward implementation of the methods described in the GUM leads to impossible and impracticable equations because of the correlations between some millions of measurement points. A practical solution is found in taking the main aspects of uncertainty, as these are given in the recent ISO 25178 standards series and apply these to a measured surface topography as a whole.

1 Introduction

In the last decades, the measurement and calibration of roughness in terms in of the well-established 1.5-D roughness parameters such as *Ra*, *Rz*, etc are well fixed in appropriate ISO standards. However a proper uncertainty evaluation is rather tedious for even the most elementary parameters, as has been shown by e.g. Morel [1], Haitjema [2], Harris [3] and Krystek [4].

The classical *R*- parameters are especially descriptive for stratified surfaces as they are produced by most machining processes. However for a general surface these fail as it is recognized that surfaces are essentially 2.5-D. With 2.5-D is meant that an equidistant *x*-*y* grid is projected on a surface, and the surface can be completely described by attributing one *z*-coordinate to every *x*,*y* coordinate. The uncertainty estimation of 2.5-D parameters (i.e. the *S*-parameters according to ISO 25178-2:2012 [5]) is somewhat more complicated but can be basically carried out in a similar manner. The basis for an uncertainty estimation must be the metrological characterisation of the surface measuring instruments and its specification. Recently the way these instrument as well as the measurement conditions should be specified was redefined in the ISO 25178 series, where all surfaces and instrument are described as basically areal, and the *R* parameters and their measuring instrument are considered as a sub-set of more general areal *S*-parameters measuring instruments. As the specifications basically aim to describe aspects that determine measurement uncertainties (better specifications should mean lower measurement uncertainties), in this paper the newest specifications as standardized will be taken as a basis for some examples of uncertainty estimations.

2 Changes in ISO 25178-series compared to ISO 3274

The standard ISO 3274:1996 [6] describes as the title says: nominal characteristics of contact (stylus) instruments. It describes e.g. the 0.75 mN measurement force, the nominal probe tip radius of 2 µm, and how this relates to the cut-off wavelengths, the bandwidth and the maximum sampling spacing.

A clear limitation is in table 1 of this standard: the smallest short-wavelength cut-off length λs is 2.5 µm, implying that that at smaller scales no roughness can be measured. This limitation has clearly been eliminated in ISO 25178-3 [7], where table 1 from ISO 3274 is extended to larger and smaller scales in table 2, and a similar table 3 is presented for optical measurement. Further the bandwidth is defined in table 1, with a minimum value of 1:100, where in ISO 3274 the minimum value was 1:30. The long-wave cut-off wavelength λc is now called the L-filter nesting index, the short-wave cut-off wavelength λs is called the S-filter nesting index and the long-wavelength can also be omitted and replaced by the form, it is called the F-operation index, and can e.g. consist of removing the least-squares plane. The requirement, or at least strong advice, in ISO 4288:1996, to measure 5 cut-off lengths λc, is dropped. A further essential point is that the default surface is defined as the mechanical surface. As the spacing and probe diameter are defined as maximum values in ISO 25178-3, table 2, this means implicitly that the measurement bandwidth should be determined purely by the filtering characteristics, with the probe diameter, spacing and measuring force taken as small enough as to have no further influence. This means:

The probe diameter shall be so small that it does not affect the measurement. For a finite probe size the deviation this gives should be corrected or quantified as a contribution to the uncertainty.

The spacing shall be small enough as not to affect the measurement (i.e. parameter value). For a finite spacing the deviation this gives should be corrected or quantified as a contribution to the uncertainty.

The probing force shall be so small that it does not affect the measurement. For a finite force the deviation this gives should be corrected or quantified as a contribution to the uncertainty.

3 Quantifying influencing uncertainties

Of course one can – and should – use common sense to determine which uncertainty contributions should be taken into account for which quantity. However the ISO 25178 series has determined influencing factors for every type of instrument that should be taken into account, at least as a kind of checklist. For every measurement instrument there is the general ISO 25178-600 [8], that gives a basic table (again 'table 1'). Table 1 in ISO 25178-600 lists aspects that are relevant for any measurement method such as linearities in x, y, and z, measurement noise, etc. In addition to this, ISO 25178-601 [9], that list specific requirements for contact instruments may be considered, especially its table 1 where tip radius is mentioned, and further ISO-25178-3 as far as the ideal conditions (negligible probing force, spacing and tip radius) are not met.

On the other hand, if e.g. a white-light interferometer measurement is considered, one should consider the same ISO 25178-600 table 1, plus ISO 25178-604 [10] which however gives no different aspects as already covered in ISO 12178-600, and ISO 125178-3 table 3 for sampling distances and period limit.

Obviously, the relevance of these factors depends on the parameter: the z-axis linearity and amplification is most relevant for amplitude parameter like *Sa*, while the x-axis linearity and amplification is most relevant for a spacing parameter like *RSm* or *Sal*. In this section the direct and indirect influencing factors are discussed. This distinguishes how these factors can be quantified and to what extent these are task-specific; i.e. they depend on the geometry of the specimen measured.

3.1 Direct influencing instrumental factors

As direct influencing factors, the instrumental geometric deviations are considered that directly influence the parameter quantity. This factor depends on the parameter definition, especially its unit and the meaning of that unit. An example is the parameter *Sa*, that is the average deviation in the z-direction. It is important to be aware of the fact that the unit 'µm' in which this parameter is expressed refers to the ordinates of the coordinate points, usually taken in the z-direction. Therefore also the noise in the definition direction(s) is a direct influencing factor. As a direct influencing factor of the second kind, geometrical deviations of other scales in the direction of the defined parameter are considered, e.g. the translational (straightness) deviations of the x- and y- axes in the z-direction, *yTz* and *xTz* are relevant for the *Sa* parameter. In ISO 12178-600 these effects are summarized as 'residual flatness'. These influencing factors of the second kind depend on the area and range in which the *x*- and *y*-axes are used in a measurement.

3.2 Indirect influencing instrumental factors

Indirect influencing factors are factors that do not relate to the principal unit of the parameter, but influence the parameter value via the definition and the inability to satisfy this definition precisely. Indirect influencing factors of the first kind are calibrations of the axes that are not directly part of the parameter definition but can come in this definition indirectly because of filtering or other parts of a definition. The calibration of the x- and y- axes and their squareness in the case of the *Sa* parameter are examples. Indirect factors of the second kind are factors that appear as a definition that cannot be realized precisely. Typical examples are the sampling frequency that cannot be infinite (or cannot meet the requirements given in ISO 25178-3), the probe size (it cannot be infinitely small or cannot meet the requirement as given in ISO 25178-3), and the measurement force (that cannot be zero). For optical measurements these are also the effects that make the optically measured surface not coincide with the mechanical surface, such as dissimilar materials, thin films, phase shifts, etc., as the mechanical surface is defined as the standard in ISO 25178-3-section 4.2.2.

3.3 Specimen effects

As is generally known, very different specimen geometries can give a same roughness parameter. However this geometry determines the relevance of the indirect influencing factors as mentioned in section 3.2. A separate specimen effect is the homogeneity of the parameter over the surface, in the cases where the exact measurement location on the surface is not specified. In many cases the inhomogeneity of the surface is the dominant factor that affects the uncertainty. This is the more the case where *S*-parameters are no more defined as the average of 5 consecutive cut-off length, as the *R*-parameters. This not only omits some statistical averaging, but moreover it replaces a well-defined Gaussian filtering by an oddly-defined one (any longer wavelengths than the cut-off length appear as high frequencies due to the folding effect) and/or a least-squares fit that is much more sensitive to the measured geometry. This all highly degrades the measured surface inhomogeneity, and, through that, the uncertainty in a parameters that characterizes a whole surface.

2.4 Software effects

Although the parameters and filtering are defined in standards, there is quite some room for interpretation and implementation (see e.g. Leach [11]). An example is the issue whether coordinates can just be translated when referring to a reference plane or the coordinate system should be rotated (see Senin [12]). Serious efforts are made to come to harmonization in this respect (Harris, [13]).

4 Method of uncertainty estimation

In the recent years, the methods of uncertainty estimation has been largely established and fixed. The basic documents are the GUM (ISO/IEC Guide 98-3) [14] and it's 'Supplement 1' (ISO/IEC Guide 98-3/Suppl 1) [15]. In the GUM the analytical method is described where the calculation can be summarized in an uncertainty budget, as specified in EA-4/02 [16]. The Annex 1 document describes the more general approach that is focused on the propagation of uncertainty distributions rather than values, and out of their nature, Monte-Carlo methods are the only practical approach for this. In an earlier paper the equivalence of these approaches was illustrated [17].

Basis for any uncertainty is the model function that relates the output quantity Q to the input quantities p_i. An estimate of the measurand Q, the output estimate denoted by q, is obtained from equation (1) using input estimates p_i for the values of the input quantities P_i:

$$q = f(p_1, p_2, ..p_N) \tag{1}$$

(here the commonly used symbols x and y are not used to avoid confusion with the x- and y-axes in this paper). For the case of 2.5D roughness parameters this looks attractive at first sight, as at least some roughness parameters are defined in ISO 25178-2 in a form similar to (1), for example Sa:

$$Sa = \frac{1}{A}\iint_A |z(x,y)|\,dxdy \approx \frac{1}{n_x \cdot n_y}\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}|z(x_i, y_j)| \tag{2}$$

Now, when taking the formalism to calculate the standard uncertainty $u(Sa)$ even this simplest example already becomes rather cumbersome:

$$u(Sa)^2 = \sum_{i=1}^{n_x}\sum_{j=1}^{n_y}\left[\frac{\partial(Sa)}{\partial z(x_i, y_j)}u(z(x_i, y_j))\right]^2 + 2\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}\sum_{k=1}^{n_x}\sum_{l=1}^{n_y}\frac{\partial(Sa)}{\partial z(x_i, y_j)}\frac{\partial(Sa)}{\partial z(x_k, y_l)_{i,j\neq k,l}}u(z(x_i, y_i))\cdot u(z(x_k, y_l)) \tag{3}$$

Here the second term denotes the correlations. With a, rather limited, x,y grid of 100 x 100 points, the correlation matrix already consists of 10^8 terms. In most common uncertainty calculation the correlations can be neglected, but here the z-values are highly correlated; e.g. by the probing process, by the filtering process, by a common calibration factor, etc.

With the implicit and explicit measurement conditions, filtering- and evaluation methods, also (2) is far too simple, in fact if Sa_d is the Sa as it is defined, and Sa_m how it is measured, (2) can be rewritten as:

$$Sa_d = \frac{1}{A}\iint_A \left|S\left(F_F(z(x,y)\right)\right|; \quad Sa_m = \frac{1}{n_x \cdot n_y}\sum_{i=1}^{n_x}\sum_{j=1}^{n_y}\left|S\left(F_F\left(F_D\left(z(x_i, y_j)\right)\right)\right)\right| \tag{4}$$

Here F_D is the dilation function that convolutes the real surface with the probe form (see e.g. Soile [18]) and the elastic deformation, F_F is the form removal function that subtracts the least-squares plane from the measurements, and S is the S-filter, e.g. the Gaussian filter according to ISO 16610-21:2011 [19]. Sa_d can be considered as the value of Sa_{m} in the limit of zero measurement force, zero probe diameter and zero sampling distance. Obviously these requirements cannot be met, but at least the uncertainty estimation should incorporate these factors in such a way that the Sa_d value can be expected to be inside the uncertainty interval attributed to Sa_m.

The functions F_F and S can be given in numerical/analytical form, but we will spare the reader writing (4) in a more explicit form. What is important here is that the *Sa* function, or any other parameter, will be considered as a result of a complex measurement, convolution, transforming, filtering and calculation process that gives a numerical value, the *Sa* parameter, in the end.

What can be done however, provided the real profile, probe diameter and the filter settings are known, is finding out the sensitivity of the *Sa* parameter to factors like probe diameter, deviations in the measured coordinates, noise, flatness deviation, and all the aspects that are mentioned in the standards. In that case it can be calculated numerically how the *Sa*-value varies with these parameters. In this case, the uncertainty can be calculated as:

$$u(Sa)^2 = \sum_{p=1}^{n} \left[\frac{\partial (Sa)}{\partial p} u(p) \right]^2 \tag{5}$$

Here p denotes the influencing parameter, e.g. the S-filter with $\lambda_s = 2.5$ µm, $u(p)$ is the uncertainty in the parameter, or the (expected) deviation from nominal, e.g. $u(\lambda_s) = 0.5$ µm and *Sa* is the *Sa* parameter that is the result of all the operations in (4).

For all influencing factors p, (5) can be approximated by:

$$u(Sa)_p = \left| Sa_{p=nominal} - Sa_{p=nominal+uncertainty\ \ or\ \ deviation} \right| \tag{6}$$

In (5) and (6) it is assumed that the influencing parameters are not correlated. This is not completely true; e.g. the S-filter will correlate with the probe diameter if these have a similar filtering effect, however it will be close enough.

For directly influencing instrumental factors, equation (6) is rather trivial, e.g. if the calibration factor of the z-axis has an uncertainty of 1%, the uncertainty in the *Sa* parameter will be 1% as well. For indirect influencing instrumental factors this relationship is far less trivial and in order analyze all indirect influencing factors according to (6), a user ideally would know the real areal geometry and have software that can filter, convolute, deconvolute, etc. If the real surface is known, of course no more uncertainty analysis is needed. However measurement data that approximate the real surface geometry can well be used to estimate most influencing factors. In figure 1 it is illustrated how this can be done in the case of a finite-size probe. As the measured surface is a convolution of the real surface with the probe, the real surface can only be estimated as a de-convolution of the measured profile with the estimated probe geometry. This estimated 'real surface' can then subsequently be convoluted with a nominal (or no) probe, and with a deviating (or estimated) probe size. For the 1.5-D case this was illustrated earlier [17]. The difference in the *Sa* parameter of both surfaces is then an estimate of the uncertainty due to probe influences. In a similar way an uncertainty due to a filtering effect, (or the measurement force, etc), can be estimated when only a filtered profile is available.

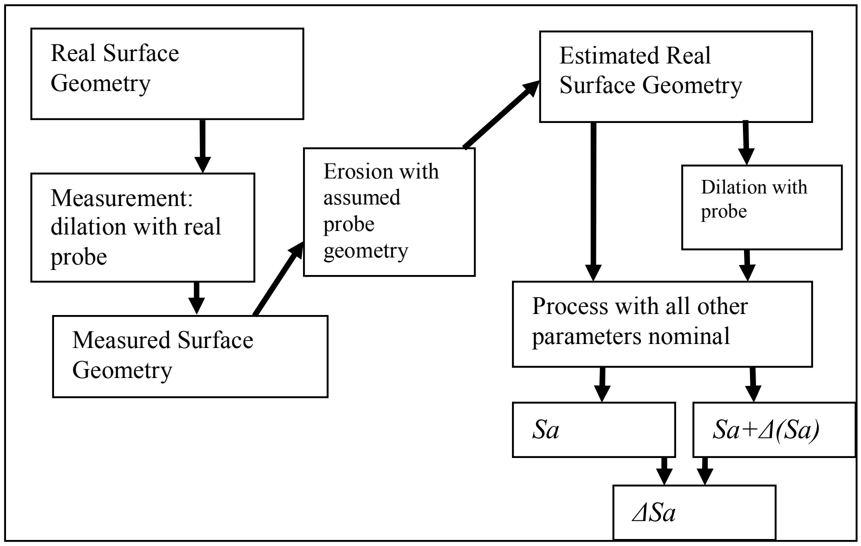

Figure 1 Schematic of uncertainty estimation due to probe size

5 Relevant influencing factors in an uncertainty estimation

As an example of how different aspects should be considered, 3 different parameters are considered: in 1.5-D a *Ra* value of a periodic structure, a *Ra* and a *RSm*-value of a type-D specimen and in 2.5-D a *Sa*-value of that same type-D specimen.

Table 1: Qualitative summary of expected influencing factors for different parameters on different specimen

ISO Standard	factor	*Ra*, periodic	*RSm* type D	*Sa* type D
25178-600	Amplification α_x	Indirect, first kind	Direct, first kind	Indirect, first kind
25178-600	Amplification α_y	-	-	Indirect, first kind
25178-600	Amplification α_z	Direct, first kind	Indirect, first kind	Direct, first kind
25178-600	Linearity l_x	Indirect, first kind	Direct, first kind	Indirect, first kind
25178-600	Linearity l_y	-	-	Indirect, first kind
25178-600	Linearity l_z	Direct, first kind	Indirect, first kind	Direct, first kind
25178-600	Residual flatness	Direct, second kind	Direct, second kind	
25178-600	Measurement noise	Direct, second kind	Indirect, second kind	Direct, second kind
25178-600	Spatial resolution	Indirect, second kind	Direct, second kind	Indirect, second kind
25178-600	Perpendicularity x,y	-	-	Indirect, first kind
25178-601	Tip radius	Indirect, second kind	Indirect, second kind	Indirect, second kind
25178-601	Cone angle	Indirect, second kind	Indirect, second kind	Indirect, second kind
25178-3	S-filter	Direct, second kind	Indirect, second kind	Direct, second kind
25178-3	L-filter	Direct, second kind	Indirect, second kind	Direct, second kind
25178-3	Form removal	-	-	-
25178-3	Sampling distance	(see spatial resolution)		
25178-3	Tip radius: see above			
(3274)	Measurement Force	Direct,second kind	Indirect, second kind	Direct,second kind
-	Inhomogeneity	p.m.	p.m.	p.m.

The influences are quantified in table 2:

Table 2: Quantitative uncertainty budget for the 3 parameters discussed.
Contributions < 0.1% are omitted.

ISO Standard	factor	*Ra* = 3 µm	*RSm* = 16 µm	*Sa* =120 nm
25178-600	Amplification α_x (1%)	0	0.5%	0
25178-600	Amplification α_y (1%)	-	-	0
25178-600	Amplification α_z (1%)	0.5%	0	1%
25178-600	Residual flatness (0.040 µm for x-axis, 0.33 µm for x-y plane)	0	0.3%	2.5%
25178-600	Measurement noise (*Rq* = 16 nm)	0	0.3%	1%
25178-600	Spatial resolution (0.5 µm →1 µm)	0	8%	1%
25178-601	Tip radius	0.2%	0.7%	2%
25178-3	S-filter	0	0.7%	1%
25178-3	Form removal	n/a	No	No
Total, standard uncertainty		0.6%	9%	4%

Note that the uncertainty in the *Ra*-value of a periodic specimen is exclusively determined by the z-calibration (amplification). This makes such a specimen very appropriate to calibrate the z-amplification α_z. For the other parameters in this example, other factors are more important.

6 Conclusions and discussions

The elements that should be part of an uncertainty calculation of 2.5-D roughness parameters are given, based on recent and draft ISO-standards. The uncertainty-budget method as presented here can be replaced by a Monte-Carlo method, which gives the same results, but it gives little insight, that is why it is omitted here. It is shown that for the simplest amplitude parameters this is already a tedious exercise; however the major factors are the z-calibration and the reference plane/noise contributions that can well be estimated in general. As expected for a periodic profile only the z-calibration factor is relevant, therefore these standards can well be used to calibrate the z- (and x-) axes. For random-like standards the uncertainty contributions are more mixed; in this case the tip radius and residual x-y flatness (for *Sa*) and the spatial resolution (for *RSm*) contributed more to the uncertainty than the basic axes calibration, illustrating that the traceability of surface roughness measurement is more complicated than just the calibration of the linear axes.
Once the use of 2.5-D parameters becomes more common, the question about the uncertainty in these values will appear automatically, and then the methods described in this paper may form a good starting point for a proper evaluation.

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