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Uncertainty propagation of field areal surface texture parameters using the metrological characteristics approach

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Abstract

The ISO 25178 series of specification standards describes the nominal characteristics of and calibration methods for areal surface topography measuring instruments. These standards also summarise the influence factors that contribute to the measurement uncertainty of each type of instrument. Due to the variety and complexity of these factors, uncertainty evaluation of surface topography measurements can be complex. The metrological characteristics (MCs) framework combines the different influence factors into a set of characteristics that can be measured with relative ease. Once determined, MCs can be propagated through an appropriate measurement model to evaluate the uncertainty in some measured quantities, in accordance with the methodology found in the *Guide to the Expression of Uncertainty in Measurement* (GUM). Hence, the combined standard uncertainty is evaluated by addition in quadrature of the product between the standard uncertainty for each metrological characteristic and their respective sensitivity coefficient. This approach is a modified version of the GUM framework, where the input quantities are considered as independent, and the influence of the MCs is treated as a type B uncertainty. In this work, we present the development of software that can calculate the sensitivity coefficients for different surface texture parameters, propagate the MCs through an appropriate measurement model and, ultimately, output the uncertainty in a surface texture parameter for a given surface. The software can be used for the evaluation of all areal field parameters found in ISO 25178 part 2. Within the context of this software, the standard uncertainty contribution due to the topography fidelity MC is considered to be the difference between the measured and a reference surface for each field parameter, after the other MCs have been adjusted or otherwise considered.

advanced manufacturing, metrology, metrological characteristics, uncertainty

1. Introduction

The metrological characteristics (MCs) framework, introduced in ISO 25178 part 600, combines different influence factors that contribute to the uncertainty of a measurement into a list of seven explicitly stated characteristics [1]. These characteristics, when propagated through an appropriate model, allow for the evaluation of uncertainty for a measured quantity [2]. The model follows the methodology outlined in the *Guide to the Expression of Uncertainty in Measurement* (GUM) [3], where the combined standard uncertainty is evaluated as the sum of the squares of the product of the standard uncertainty for each MC and their respective sensitivity coefficients.

The application of the MC methodology, though a straightforward process, requires the calculation of the different sensitivity coefficients. This process is complex, as each sensitivity coefficient is unique – it describes the variation in magnitude of a surface texture parameter with respect to changes in the values of the MCs. In this work, we have developed software that can be used for the evaluation of uncertainty for the areal field parameters as found in ISO 25178 part 2. The software calculates the uncertainty contribution for each MC using a suitable propagation function. The overall goal of this software is to simplify the process of evaluating uncertainty in surface texture measurement for those working in industry and research.

2. Methodology

Following the methodology outlined in the GUM [3], the combined standard uncertainty is calculated as a combination of type A and type B standard uncertainty components. The difference between the method for evaluating uncertainty between the two, is that type A uncertainty is evaluated by statistical analysis of a series of observations, while type B is evaluated using any other means, e.g. evaluating the amplification coefficient using a number of step height material measures. The uncertainty components attributed to the MCs are treated as type B uncertainties, since the default methods for evaluating the MCs are not based on frequency distributions. Moreover, it is assumed that there is no correlation between the influence factors. The combined standard uncertainty is calculated as follows:

$$u_B^2 = \sum_{i=1}^{n} (c_i)^2 \, u_i^2, \qquad (1)$$

where u_B is the combined standard uncertainty, c_i are the sensitivity coefficients for each MC's contribution and u_i are the uncertainty contributions for each MC. The evaluation of the standard uncertainty is restricted to the most relevant MC for which the uncertainty can be evaluated. For example, the uncertainty for a surface height parameter, such as *Sq* [4], does not have any significant influence from the amplification and linearities in *x* and y (instrument measurement axes). Table 1 lists the MCs along the major axes they influence. The categorisation of the primary influence found in table 1 assumes good measurement practice for the determination of the MCs, according to the National Physical Laboratory (NPL) good practice guides (for example, see [5]).

Table 1 List of the metrological characteristics and the measurement axes they influence, respectively.

Metrological characteristic	Symbol	Influenced axis/axes
Measurement Noise	N_M	*z*
Flatness deviation	z_{FLT}	*z*
Amplification coefficient	a_x, a_y, a_z	*x, y, z*
Linearity deviation	l_x, l_y, l_z	*x, y, z*
x-y mapping deviations	$\Delta_x(x,y)$, $\Delta_y(x,y)$	*x, y*
Topographic spatial resolution	W_R	*z*
Topography fidelity	T_{Fi}	*x, y, z*

It should be noted that, at the time of writing, the MCs of topographic spatial resolution and topography fidelity do not have a default method of evaluation. The influence of topographic spatial resolution can be quantified according to the guidelines found in VDI/VDE 2655 part 1.3. The suggested material measure contains gratings of various periods, with rectangular cross sections and of the same height [6]. VDI/VDE 2655 part 1.3 also suggests a method for evaluating the uncertainty due to topography fidelity, solely for profile measurement. In VDI/VDE 2655 part 1.3, the term is denoted as profile fidelity and is defined as the *'description of how well two-dimensional structures can be reproduced by a measurement'*. The suggested material measure for evaluating profile fidelity is characterised by either sinusoidal or rectangular profiles. As in the topographic spatial resolution case, a comparison is made between the measured profile and a calibrated model profile, after appropriate pre-processing is carried out. The effect of lateral resolution is excluded by filtering the two profiles accordingly [2,7].

3. Uncertainty propagation software

The uncertainty propagation software allows the user to evaluate uncertainty for the different field parameters described in ISO 25178 part 2 [4]. The method for evaluation of measurement uncertainty that the software uses is a modified approach to the GUM methodology, based on work performed by Haitjema [7], and involves a recalculation of the full topography, while varying the MCs and considering the variation of the field parameters. The architecture of the software is illustrated in Figure 1.

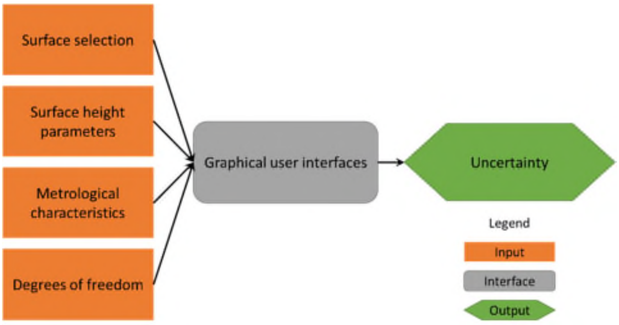

Figure 1 Uncertainty propagation software architecture.

In figure 1, the rectangular nodes denote the input parameters to the software:

- Surface selection: corresponding to the profile or areal (every *x* or *x-y* coordinate defines one height coordinate) [7] height map data of the measured topography.
- Surface field parameters: corresponding to the field parameters measured by the user which are used for the evaluation of the corresponding sensitivity coefficients.
- Metrological characteristics: the MCs are the main input parameters for the software in order to evaluate uncertainty.
- Degrees of freedom: the degrees of freedom for each MC are used to determine the effective degrees of freedom for the calculation of the expanded uncertainty.

The round node represents the graphical user interfaces with which the user interacts while using the software. Finally, the hexagonal node refers to the output of the software, which is the combined standard and expanded uncertainties. The user can also access the individual uncertainty contributions for the combined standard uncertainty.

4. Uncertainty propagation for the surface parameter *Ssk*

An example uncertainty budget is given for a sinusoidal material measure (nominal wavelength, *RSm* = 50 µm and nominal amplitude, *Pt* = 1.5 µm) as seen in Figure 2 below. The measurements were performed using a coherence scanning interferometry (CSI) instrument and the measurement uncertainty is evaluated for the areal field parameter of skewness (*Ssk*). The instrument used to carry out the measurements is a Zygo NewView NX2, fitted with a 50× magnification objective whose specifications can be found in Table 2.

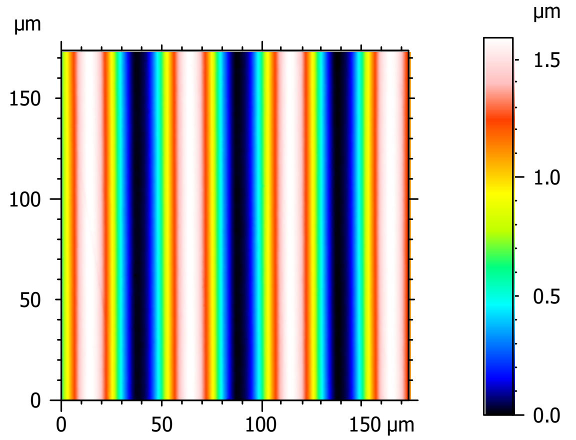

Figure 2 Example surface topography measurement of the sinusoidal artefact using CSI.

Table 2 Objective specifications for the CSI instrument

50× objective specifications	
Numerical aperture (NA)	0.55
Optical resolution	0.52 µm
Field of view (FOV)	0.17 mm
Spatial sampling	0.17 µm

The *Ssk* parameter is a measurement of the symmetry of the surface deviations about the mean reference plane and in its discrete form is given by the following equation:

$$Ssk = \frac{1}{Sq^3 N}\sum_{i=1}^{N} z_i^3, \tag{2}$$

where *Sq* corresponds to the root mean square of the ordinate values, z_i within the sampled topography. *N* is then the total number of measured height values and z_i are the measured height coordinates. Combining equations (1) and (2) to arrive at an expression for the propagation of uncertainty for the *Ssk* parameter, we find:

$$u_{Ssk,p}^2 = \left(\frac{3}{NS_q}\right)^2 \sum_{i=1}^{N}\left[\frac{z_i^2}{Sq^2} - 1 - \frac{Ssk}{Sq} z_i\right]^2 (u_{i,p})^2, \tag{3}$$

where the left hand side of equation (3) corresponds to the sensitivity coefficient for the *Ssk* parameter. As *Ssk* is a height parameter, it is primarily influenced by the MCs of measurement noise, flatness deviation, amplification and linearity in the *z* axis, topographic spatial resolution and topography fidelity. Consequently, assuming good measurement practice, the contribution of the other MCs is negligible and can be safely omitted. The measurement noise contribution is independent of the values of the measured height coordinates. As such, the equation for evaluating the contribution of measurement noise to the measurement uncertainty of the *Ssk* parameter is given by:

$$u_{Ssk,N_M}^2 = \left(\frac{3u_{i,N_M}}{NS_q}\right)^2 \sum_{i=1}^{N}\left[\frac{z_i^2}{Sq^2} - 1 - \frac{Ssk}{Sq} z_i\right]^2. \tag{4}$$

Following the NPL good practice guide [5], the measurement noise was evaluated using the subtraction method as u_{i,N_M} = 0.81 nm. Inserting the value into equation (4) along with the values for the other parameters (*N* = 1,000,000, *Sq* = 0.558 µm and *Ssk* = -0.196), yields u_{Ssk,N_M} = 0.003. To verify the results, a repeatability test was carried out over five repeats of the topography at the same location, yielding a standard deviation of 0.0005 for the *Ssk* parameter, which is consistent with the results obtained from equation (4). As residual flatness is also independent of the measured *z*-axis coordinates, the following equation is used to determine its uncertainty contribution

$$u_{Ssk,Z_{FLT}} = \sqrt{Ssk^2 + u_{i,Z_{FLT}}^2} - Ssk. \tag{5}$$

Equation (5) is a comparison between the *Ssk* parameter of the measured topography for the sinusoidal material measure before and after superimposing the flatness map onto it. The flatness map (as seen in Figure 3) is a height map that is used for the quantification of the MC of flatness deviation. The comparison shows that $u_{Ssk,Z_{FLT}} = 0.000003$, which is negligible.

A total of four step height material measures, covering the working range of interest (*Pt* = 1.5 µm), were used to determine the uncertainty contribution for the amplification coefficient. Each material measure was measured at each location five times and, using the analysis method outlined in ISO 5436 part 1, the mean depth of each material measure was evaluated as seen in Figure 4.

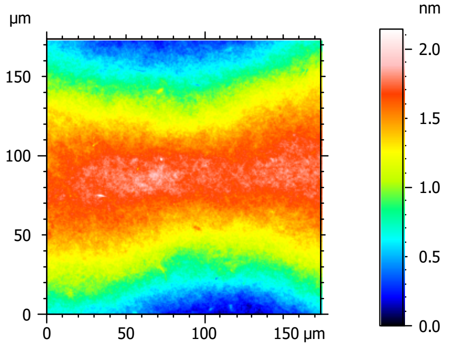

Figure 3 Residual flatness topography map.

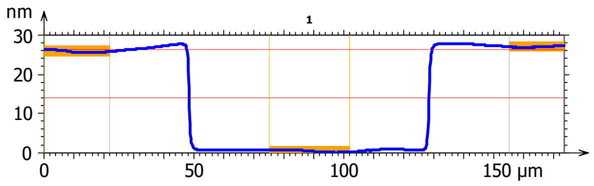

Figure 4 Step height material measurement analysis example for a step height material measure of the nominal height of 25 nm.

From the NPL good practice guide, the measurement uncertainty for the amplification coefficient is evaluated as the combined effect of four terms:

$$u_a = \sqrt{u_{error}^2 + u_{repeat}^2 + u_{repro}^2 + u_{trac}^2}, \tag{6}$$

where:

- u_{error} is the measurement error: the difference between the measured value and nominal value for a step height/depth material measure;
- u_{repeat} is the repeatability error: the maximum standard deviation of the mean depth value calculated at each position;
- u_{repro} is the reproducibility error: the standard deviation of the average depth values at each of the measured positions; and
- u_{trac} is the traceability error: the contribution from the calibration of the step artefact, determined using an instrument traceable to the formal definition of the metre.

As the amplification coefficient is a ratio of the measured height values to the nominal height values, it is proportional to said height values, so that $u_{i,a} = u_a z_i$. Replacing the $u_{i,a}$ parameter in the propagation function of the *Ssk* parameter, the uncertainty contribution of the amplification coefficient is given by:

$$u_{Ssk,a}^2 = \left(\frac{3u_a}{NS_q}\right)^2 \sum_{i=1}^{N}\left[\frac{z_i^2}{Sq^2} - 1 - \frac{Ssk}{Sq} z_i\right]^2 (z_i)^2. \tag{7}$$

It should be noted that equation (6) also contains the uncertainty contribution for the MC of linearity deviation. Using the data found in Table 3 and equation (6), results in u_a = 0.079, which gives $u_{Ssk,a}$ = 0.052.

Table 3 CSI z-axis scale calibration results

Nominal height /nm	25	200	500	1000
u_{err} /nm	1.06	0.98	2.75	79.37
u_{repeat} /nm	0.21	1.42	0.39	0.55
u_{reprod} /nm	2.47	0.95	1.13	2.54
Traceability /nm	2.9	2.9	2.9	2.9

The topographic spatial resolution and topography fidelity contribution can be evaluated following the VDI/VDE 2655 part 1.3 guidelines. In detail, a profile is extracted from the CSI measurement and compared to a representative profile measured in the same area using a traceable stylus instrument. After appropriate postprocessing, which involves alignment of the two profiles, levelling and filtering, the uncertainty contribution of topographic spatial resolution is evaluated as the difference of the *Ssk* parameter resulting from the difference between the two profiles. The profile fidelity contribution is evaluated using the same profile but with an application of an additional S-filter nesting index so that the effect of lateral resolution is removed. As the optical resolution of the objective is given at 0.52 µm from the data of Table 2, the S-filter used is 0.6 µm. After the application of the filter, the difference profile is used to quantify the contribution of fidelity for the *Ssk* parameter. As comparison to a stylus instrument was not feasible and as such representative values were given for the uncertainty contribution for topographic spatial resolution $u_{Ssk,r}$ = 0.00011 and topography fidelity $u_{Ssk,f}$ = 0.0002. Having evaluated the uncertainty contribution for each of the MCs, inserting their values in equation (1), the combined standard uncertainty is evaluated as

$$\begin{aligned} u_{Ssk}^2 &= u_{Ssk,N_M}^2 + u_{Ssk,Z_{FLT}}^2 + u_{Ssk,a}^2 + u_{Ssk,r}^2 \\ &\quad + u_{Ssk,fi}^2 \\ &= (0.003)^2 + (0.000003)^2 + 0.0052^2 \\ &\quad + 0.00011^2 + 0.0002^2 \\ &= 0.000027, \end{aligned}$$

so

$$u_{Ssk} = 0.006.$$

An overview of the uncertainty budget for the *Ssk* parameter can be found in Table 4. The expanded uncertainty is calculated by multiplying the combined standard uncertainty by a coverage factor, representing a certain confidence interval which is usually 95 %. To determine the coverage factor, the Welch-Satterthwaite equation is used to approximate the effective degrees of freedom of the independent influence quantities.

$$v_{eff} = \frac{u_B^4}{\sum_{i=1}^{N} \frac{u_i^4}{v_i}} \cong \infty. \qquad (8)$$

As all of the uncertainty contributions of the MCs are considered as type B uncertainties with known values it can be assumed that $v_i \to \infty$. Consequently, the denominator of equation (8) approaches 0 and as a result the effective degrees of freedom approach infinity. Using the t-distribution table found in the GUM it is found that the coverage factor is 1.96. Finally, the expanded uncertainty for the *Ssk* parameter for a 95 % confidence interval is

$$Ssk = -0.196 \pm 0.012.$$

Table 4 Uncertainty budget for the *Ssk* parameter. The sources of uncertainty are included along with their deviation and their effect on the Ssk parameter.

Source of uncertainty for the *Ssk* parameter	Uncertainty contribution
Noise	0.003
Flatness deviation	0.000003
Amplification coefficient & linearity deviation	0.0052
Lateral resolution	0.00011
Profile fidelity	0.0002
Standard uncertainty	0.006

5. Conclusion

Software is presented that can be used for the uncertainty propagation of the surface texture field parameters using the metrological characteristics approach. Uncertainty evaluation is carried out using a modified version of the GUM framework, where the input parameters are independent and are treated as type B uncertainty components.

An example uncertainty budget is given for the surface height parameter *Ssk*. Each of the MCs was determined using the default methods outlined in the NPL good practice guide and were propagated using the appropriate equations. Finally, the combined standard uncertainty was multiplied with a coverage factor to give the expanded uncertainty for the *Ssk* parameter.

The evaluation of uncertainty for a measured quantity is a complex task which involves identification of the influence quantities, calculation of their respective sensitivity coefficients and, finally, propagation through an appropriate measurement model. The software simplifies this process, allowing the user to evaluate uncertainty for a given surface measurement.

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