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Towards task-specific uncertainty assessment for imaging confocal microscopes

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Abstract

The traceability assessment and error budgeting of surface measurements is still an open issue for 3D microscopes and profilometers employing diverse optical measuring techniques. Moreover, the task-specific uncertainty evaluation regarding specific geometrical features is a non-covered topic as the calibration of these complex measuring instruments is still being industrially deployed, and there is a lack of tools for this aim. Hence, the manufacturing and quality control of such geometries is not metrologically controlled.

The contribution of this research aims to cover this gap by propagating calibration results of confocal imaging microscope into the task-specific uncertainty assessment. This is addressed by simulation strategies. The analyzed case studies introduce the dimensional characterization and task-specific uncertainty assessment of demanding industrial samples with nanometric structures. A periodic grating and a circular profile have been studied as representative and common dimensional features. The simulation is based on the Montecarlo approach, where 10000 measurements and their processing are iteratively performed. Adding uncertainty values to input measurement coordinates and through statistical assessment of output results, the desired uncertainty values are achieved.

The results of the study will aid in quantifying, understanding, and improving the dimensional quality control of industrial samples and therefore adjust the tolerance zone of corresponding manufacturing processes.

Task-specific uncertainty, confocal imaging, calibration, Montecarlo simulation

1. Introduction

Optical microscopy techniques such as focus variation microscopy, interferometry, and confocal microscopy are increasingly applied in research and industry as they have many advantages, like non-contact areal measurements and their high resolution and precision [1,2]. Currently, several optical measuring instruments are provided with objectives with high magnification that can take measurements with high lateral resolution. Moreover, the vertical resolution in the nanometric scale driven by piezoelectric actuators. However, complex geometries still mean a challenge to these optical instruments as the measured profiles result from the interaction between light and the sample surface where not only the topography is involved but also the material optical properties and the characteristics of the optical system itself [3].

In recent years, significant efforts have been made to develop guides and standards that define the calibration procedures of this kind of optical instruments. The primary standard is ISO 25178-700, which determines and quantifies the metrological characteristics like axes' amplification coefficients, measurement noise, mapping deviations, and spatial resolution [4]. However, although these guides and standards allow quantifying the instrument's measurement uncertainty, assigning uncertainty components to each axis, there is no unique methodology to extrapolate the instruments' uncertainty values to expanded uncertainty values of actual topography measurements.

The most rigorous way to calculate the expanded uncertainty would be to propagate the uncertainty components to the type B uncertainty. The calculation of type B uncertainty is achieved by obtaining the influence coefficient of the wanted measurand, which most of the time is not a direct estimation as it requires knowing the measurand dependence of the uncertainty components.

This work presents a different approach to estimating the uncertainty of measurands by using Montecarlo simulation to model the behavior of the system uncertainty applied to the obtained topographies.

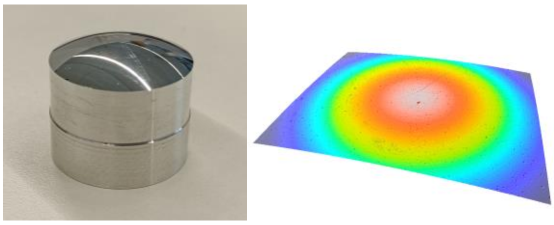
A similar approach is defined in ISO 15530-4, which establishes the guidelines for the uncertainty assessment of coordinate measuring machines (CMM) via Montecarlo simulations [5].

In this case, the Montecarlo simulation uses the optical instrument's assessed uncertainty to generate several synthetic measurements that are then statistically analyzed to extract a specific measurand and its measurement uncertainty.

2. Methods

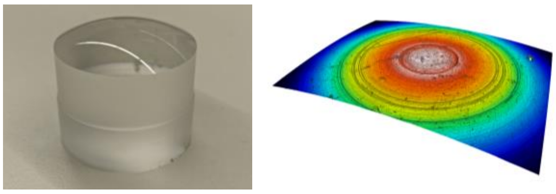
In this research, the uncertainty assessment of measurements taken with confocal imaging microscopy has been studied. The samples to characterize consist of two round surfaces and a periodic rectangular structure manufactured in a silicon wafer (Figure 3). The round surfaces were manufactured by diamond micro-turning in two different materials: Aluminum (Figure 1) and PMMA (Figure 2). The challenge of characterizing the industrial round samples was measuring their curvature radius and surface roughness. The radius measurement involves the measurable slope limit, and an appropriate objective magnification must be selected to obtain reliable results. If the magnification is too big, the measurement area could be too small to estimate the radius correctly, and a stitching of multiple measurements is requested, which may result in an overlapping error. Contrariwise, if the magnification is too low, the measured area will be enough to estimate the curvature, but the slope limit might affect the number of measured points. Therefore, a well-balanced objective selection needs to be established facing the measurement limits.

The main challenges in characterizing the periodic rectangular structures are the reduced dimensions and the vertical walls. On the one hand, the reduced dimensions demand the used objective to have enough magnification and numerical aperture to resolve the structures. On the other hand, vertical walls are usually difficult to measure with 3D optical techniques, especially for confocal microscopy. This difficulty is because this technique analyzes the reflected light from the sample's surface, and the vertical walls do not usually reflect enough light back to the instrument's image receptor.



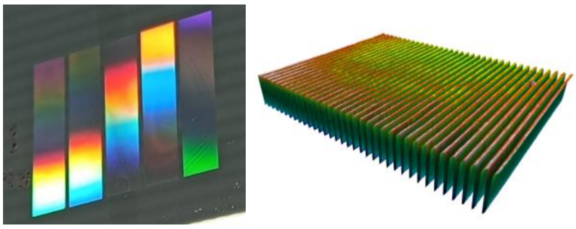
a) b)

Figure 1. Overview of the characterized samples. a) Aluminium round sample and b) 3D topography obtained with confocal imaging microscopy.



a) b)

Figure 2. Overview of the characterized samples. a) PMMA round sample and b) 3D topography obtained with confocal imaging microscopy.



a) b)

Figure 3. Overview of the characterized samples. a) Periodic rectangular sample and b) 3D topography obtained with confocal imaging microscopy.

2.1. Instrument calibration

The optical instrument proposed in this work is the SNEOX© microscope from Sensofar©, managed by SensoSCAN© software. It is an optical measuring head that unifies three measuring techniques for 3D profiling: Imaging Confocal Microscopy, Focus Variation, and Interferometry.

The instrument calibration has been carried out following the NPL Good Practice Guide (GPG 128) for the calibration of the metrological characteristics of confocal microscopes and the Guide to the Expression of Uncertainty in Measurements (GUM), permitting it to quantify every uncertainty component of the instrument [4,5]. Specifically, the uncertainty components (metrological characteristics) analyzed by these guides are the system noise, the flatness deviation, the lateral resolution of X and Y coordinates, and the linearity, amplification, and perpendicularity of the X, Y, and Z coordinates.

Each component is quantified by measuring different structures calibrated by a National Metrology Institute (NMI). The SNEOX has been calibrated using the NPL Areal Standard Set, which consists of several step height structures, siemens stars, areal cross gratings, and a flat surface. The step height structures quantify the linearity, amplification, and perpendicularity of the Z axis; the siemens stars calibrate the lateral resolution of the instrument (X and Y); the areal cross gratings assess the linearity, amplification and perpendicularity of the X and Y axes; and finally, the flat surface quantifies the noise and flatness deviation components of the Z axis.

The calibration output is the uncertainty values for each metrological characteristic, which can be combined to get the measurement uncertainty of each XYZ coordinate.

Once the system calibration was finished, the selected samples were measured with Imaging Confocal Microscopy and a 50x brightfield objective. Then, the 2D profiles were extracted from the 3D measurement to perform the task-specific uncertainty assessment exercise.

2.2. Montecarlo simulation

Figure 4 depicts the workflow of the uncertainty assessment using the Montecarlo simulation method and how it uses the random profile generator to simulate the instrument's uncertainty behavior permitting to assemble the results into probability distributions.

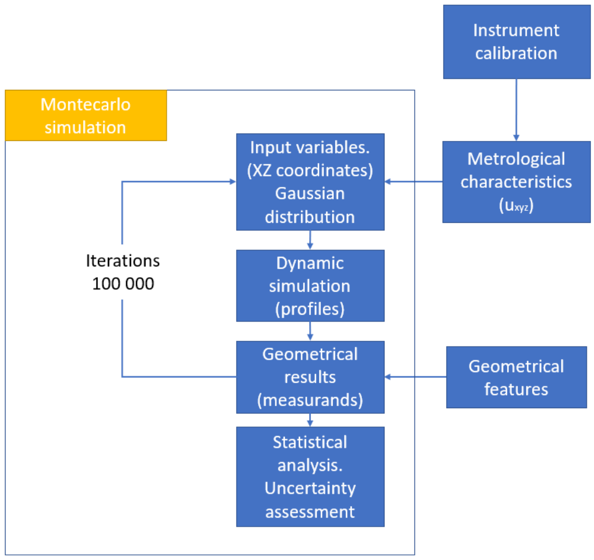


Figure 4. Schematic representation of the Montecarlo simulations' workflow applied to uncertainty assessment.

Based on the instrument calibration, an uncertainty interval is obtained for each surface point coordinate which means that the position of every surface point can be anywhere inside this interval with a degree of confidence. For example, a coverage factor of two (k=2) gives a degree of confidence of 95% for a normal distribution of the results. This is the applied criteria for the simulation algorithm. Based on a proposed profile (round or rectangular), the Montecarlo simulation approach enables to generate many synthetic profiles where every surface point is randomly shifted from the original profile position within the uncertainty interval. Then, the feature of interest was characterized by fitting algorithms for every simulated profile by two different methods, one using preliminary data for the fitting (Method 1) and the other that does not use preliminary data (Method 2). By analyzing the variation of the results, the uncertainty of the characteristic can be estimated.

In this case, the simulation environment, as well as the fitting algorithm, have been validated with a theoretical circular 2D profile, and then the uncertainty assessment of the real confocal measurements has been done both for the round and rectangular samples.

3. Results

After performing all the necessary measurements, the metrological characteristics were quantified for the SNEOX's confocal microscopy and 50x magnification objective. The resulting coordinate uncertainty is 1 micron for the X axis and 10 nanometers for the Z axis. Then, the simulation of a theoretical round profile was carried out, and as shown below, the overall procedure was validated.

Table 1. Results of the calibration of the measuring instrument.

Magnitude	Value (nm)
U_X	1000
U_Z	10

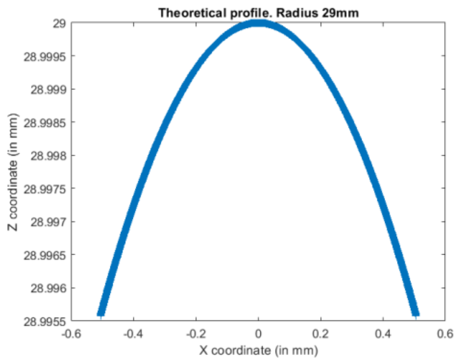


Figure 5. Proposed theoretical circular profile with a radius of 29 mm.

The selected theoretical profile has a radius of 29 mm, similar to the samples measured experimentally, to ensure that the fitting algorithms work correctly with the proposed dimensions. Then, the fitting algorithms are applied to the simulated profiles, and the statistical distribution of the radius is obtained from the results.

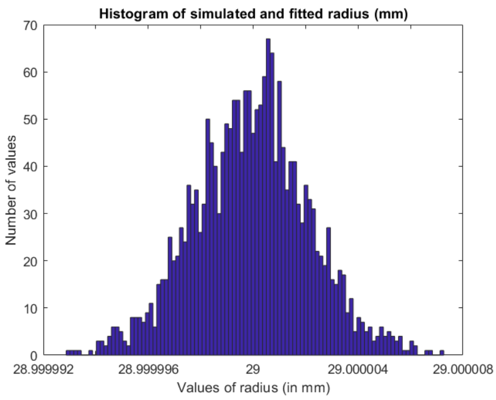


Figure 6. Statistical distribution of the fitted radius for the theoretical profile.

Figure 5 and 6 shows the simulation's verification, and it is worth noting that the histogram evidence the accuracy and precision of the fitting procedure as the standard deviation of the results for the theoretical profile is a few nanometers.

The same procedure was applied to the different 2D profiles obtained from the samples.

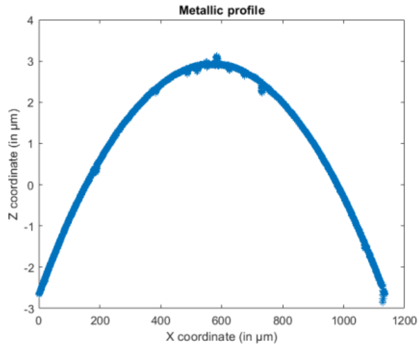


Figure 7. Measured profile of the aluminium sample.

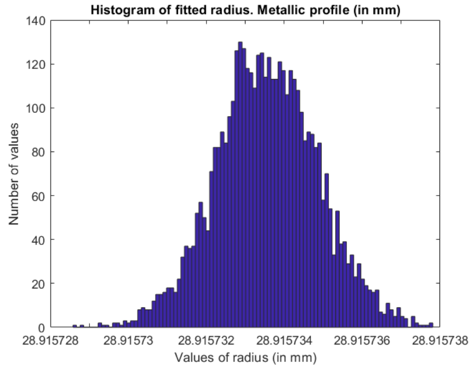


Figure 8. Statistic distribution of the fitted radius for the aluminium sample.

Figure 7 and Figure 8 show the measured profile of the aluminium sample and the statistical distribution of the fitted radius for each simulated profile. It is noticeable that the profile presents some surface defects and impurities as it has been extracted from a manufactured sample measurement. The defects on the sample surface influence the fitting process resulting in a wider statistical distribution compared to the nominal case study and, hence, a higher measurement uncertainty.

A similar procedure for data processing and uncertainty assessment has been applied for the periodic rectangular structure using synthetic data. In this case, the data processing workflow is slightly different as a primitive fitting is not requested as for the round sample case study. The processing steps are: outlier removal, edge point estimation based on spatial gradients and height/period statistical estimation based on histograms.

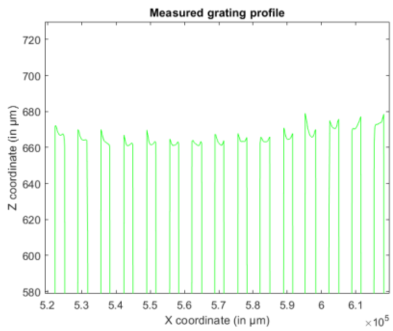


Figure 9. Measured profile of the periodic rectangular structures.

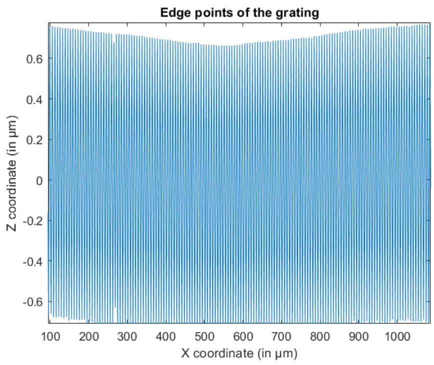


Figure 10. Edge points identified for the evaluation of the structure's height and period.

Regarding the periodic rectangular structure, a filtering of the measurement's outliers has been carried out, and as shown in Figure 10, the structure's edge points have been identified to have a reliable criterion for obtaining the characterization result. Based on the edge points, the mean period and height of the structures have been evaluated, and their standard deviation has been obtained.

Table 2. Results and statistical analysis of the radius of curvature for the round samples.

Nominal Value (mm)	Method 1 Measured Mean Value (μm)	Method 1 Std. Dev. (μm)	Method 2 Measured Mean Value (μm)	Method 2 Std. Dev. (μm)
29	28.922	2.7	28.916	2.7
27	26.905	4.1	26.723	4.1

Table 3. Results and statistical analysis of the characterized features for the periodic rectangular structures.

Characterized Feature	Nominal Value (μm)	Measured Mean Value (μm)	Std. Dev. (μm)
Height	1.5	1.462	0.04
Period	7	6.708	0.14

The numeric results of the simulations are depicted in Table 2 and

Table 3. Although the two proposed fitting methods give slightly different results for the characterized radius of curvature, the standard deviations are the same regardless of the method used. Furthermore, every calculated deviation has an acceptable order of magnitude, as no one is greater than the 5% of the characterized value.

4. Conclusion

A standardized and fast methodology is needed to assess uncertainty for 3D optical profilometers. This paper exposes a procedure for task-specific uncertainty assessment using Montecarlo simulation methods and geometrical fitting algorithms. The Montecarlo simulation approach, along with the instrument calibration uncertainty for XYZ coordinates, allows several simulation profiles to be analyzed statistically to obtain the indetermination of a particular geometrical characteristic.

From a single measurement, 100 000 profiles have been simulated, and the uncertainty associated with the radius estimation has been obtained.

It has been proved that the two fitting algorithms tried in this work converge to slightly different values. However, in the absence of reference values to estimate the system deviation, the uncertainty of the calculated values is the same regardless of the method used to characterize the sample feature.

Although this work focuses on the proposed samples, the developed procedure can be applied to any profile obtained from an instrument whose measuring uncertainty is well known. Moreover, the procedure could be extrapolated to 3D surface measurements and more complex geometries carrying out further statistical analysis of the results.

Regarding the characterization of samples, the procedure could also be applied for uncertainty assessment of surface roughness characterizations as long as the resolution and the sampling length of the measurement are appropriate to do this kind of characterization under standardized guidelines.

An even better estimation of the measurement uncertainty could be achieved if the certified characterization of the features were available. This way, it would be possible to have an estimation of the real value of every feature and verify if the presented simulation method is not only precise but also accurate enough. In addition, this certified information will provide a traceability uncertainty that would help complete the uncertainty assessment exercise.

In the future, the samples will be sent to a National Metrology Institute which will provide calibrated values of the geometrical features. This will be performed by reference measurement methods enabling to evaluate the accuracy of the developed simulation procedure.

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