MEASUREMENT UNCERTAINTY SIMULATION BY MONTE CARLO METHOD IN NANOMETROLOGY

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DOI: 10.17973/MMSJ.2019_10_2018112

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Abstract: This paper deals with determination of uncertainty and individual contributions to the measurement uncertainty on the CMM SIOS NNM-1 instrument fitted with the touch-probe scanning system Gannen XP. Manufacturer SIOS designates this machine as nano-CMM. Two non-simulation methods to determine the measurement uncertainty, the substitution and multi-position methods are addressed in detail [Sramek, Jankovych 2018]. Ruby balls with various nominal diameters are used as the measured objects. One simulation method to determine the measurement uncertainty, the Monte Carlo method, is also addressed in this paper. The paper also summarizes and specifies calculation methods to determine the measurement uncertainty, and provides results of representative sets of measurements, including determination of the expanded measurement uncertainty. This paper contains novel conclusions in the area of uncertainty measurement of nano-CMMs.

KEYWORDS

Coordinate measuring machine, measurement uncertainty, length measurement, multi-position method, substitution method, Monte Carlo method, nanometrology, ruby ball.

1 INTRODUCTION

This paper focuses on three methods used to determine the measurement uncertainty with a touch probe CMM (Coordinate Measuring Machine) SIOS NNM-1 (Nanopositioning and Nanomeasuring Machine) – hereinafter only nano-CMM.

It also includes methodology for the calculation of the measurement uncertainty and builds on the previous work of the authors [Sramek, Jankovych 2016]. This paper contains an assessment of measurement uncertainty using the Monte Carlo method, including a comparison of the results of this simulation method and both non-simulation methods, which were described in detail in previous work of authors [Sramek, Jankovych 2018].

Measurements were performed on the nano-CMM instrument, which was equipped with the Gannen XP touch probe from Xpress Precision Engineering (with diameter d_{saf} = 0.12 mm). The nano-CMM is a highly accurate coordinate measuring machine, which allows to make measurements in the range of (25x25x5) mm.

All measurements were made at the national metrology authority Czech metrology institute in Brno – hereinafter only CMI.

2 MATERIALS AND METHODS

The Nano-CMM is a measuring instrument and is also classified as a measuring system because it contains 3 laserinterferometers with their own indications as well as heat sensors and other accessories depending on the sensing system used. CMMs and nano-CMMs generally use the same calibration methods, measurements standards, and standardized methods to determine measurement accuracy. However, the design differences of nano-CMM devices, their smaller dimensions and greater accuracy create very different and high demands on the measurement process. In nanometrology, these requirements cannot be met with conventional CMM measurement standards and calibration methods.

Another significant factor in nano-CMM is the relatively wide range of sensing systems. Nano-CMMs are often equipped with scanning systems such as AFM microscopes, laser-focus sensors and interferometric sensors.

The use of these contactless scanning methods does not mean that it is a full-scale measurement of 3D space.

In these cases, the *x* and *y* axis shift are often used only to reach the target point or measurement area of the sample.

True 3D space measurement is used when using a contact scanning system equipped with a miniature ball, ie touch probe.

Therefore, when nano-CMM is being calibrated, standards suitable for use in the nanomeasurement field must be used. In practice, suitable standards of length are used that allow the realization of metrological tracebility. If such measurement standards are not available, it is necessary to select a suitable method for determining the measurement uncertainty or the accuracy measurement of the nano-CMM. In accordance with standards [ČSN EN ISO 17025: 2018, ISO 15530-3: 2004, EA 4/02 M: 2013 and TNI 01 0115: 2009] and scientific publications [Sladek 2016, Seggelen 2007] several methods were chosen to evaluate the accuracy of measurement: multi-position method, substitution and Monte Carlo method. This paper also deals with individual contributions to measurement uncertainty for all methods used. Methods for determining the measurement uncertainty are further developed and adapted to the nano-CMM system, in particular the Gannen XP-1 nano-probe measurement. The expanded measurement uncertainty was used to quantify the measurement accuracy in the nano-CMM.

2.1 Multi-position and substitution method to determine the CMM measurement uncertainty

These non-simulative methods use an uncalibrated object (multi-position) and a calibrated object (substitution) to measure. Corrected nano-CMM indication provides measurement result.

Multi-position method implements a set of measurements of the object in various positions and orientations within the nano-CMM measuring range (Figure 1).

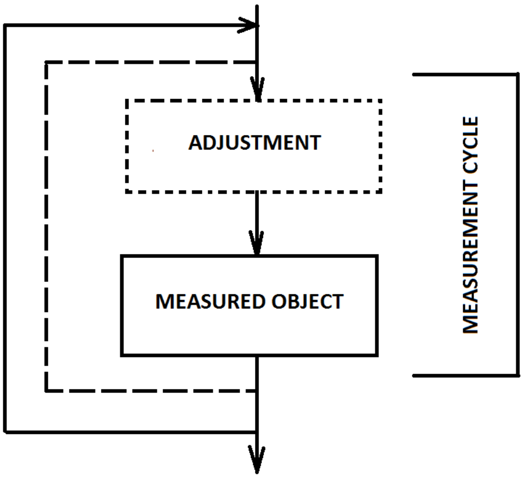

Figure 1. Scheme of the multi-position method [Sladek 2016, Sramek, Jankovych 2018]

The multi-position method [Sladek 2016, Seggelen 2007] was chosen due to the common lack of a suitable and sufficiently accurate calibration method to ensure metrological traceability of the standard used in the first phase of the measurement uncertainty evaluation.

Substitution method uses a calibrated object (standard) for the measurement (Figure 2). The uncorrected nano-CMM indication provides the measurement result.

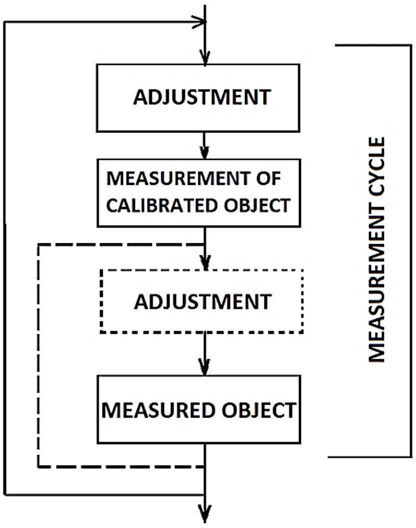

Figure 2. Scheme of the substitution method [Sladek 2016, Sramek, Jankovych 2018]

In particular, the substitution method differs from the previous method in that suitable length standards are used in the nano-CMM NNM-1 calibration process - ruby balls, which have calibration protocols with measured values and expanded measurement uncertainty. The values obtained may not be corrected by a systematic error caused by the use of an uncalibrated object. Length standards can also be used for routine measurement of nano-CMM, so they have an irreplaceable influence on the determination of expanded measurement uncertainty and the accuracy of this instrument's measurement.

2.2 Monte Carlo method to determine the nano-CMM measurement uncertainty

This method is designed to quickly estimate measurement uncertainty with reasonable reliability and reduce the burden on nano-CMM users, whether operator or metrologist. In terms of metrological tracebility of the most accurate measuring instruments and standards, the measurement uncertainty plays a crucial role. However, the reality is that the measurement uncertainty can only be analytically calculated in a simplified model case. For example, in the case of conventional CMM measurements, this is a complex spatial measurement structure where the user (operator) can arbitrarily change the measurement configuration, including the process for evaluating the measured results [Sladek 2016].

This requires a tremendous effort by the user to evaluate the measurement uncertainty, and the standard assay method is difficult to apply to complicated measurements. One limiting factor may be the limited number of measurements made for economic and time-consuming reasons. In order to solve this problem, it is possible to use the apparatus of uncertainty estimation using Monte Carlo simulation. In this paper, an accurate and simple method of estimating uncertainty using Monte-Carlo Simulation is established.

Here described methods of measuring accuracy measurement (multi-position and substitution) assume that the individual components of the standard measurement uncertainty have a stable probability distribution. The principle of the Monte Carlo method used in this paper is given in the diagram [Sira 2014] that is included in the Figure 3.

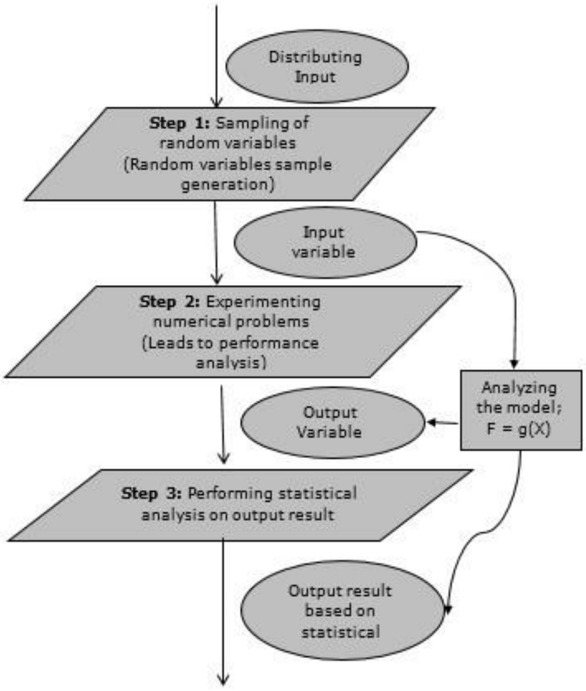

Figure 3. Scheme of the Monte Carlo method [Sira 2014]

3 USE OF SAID METHODS

3.1 Nano-CMM measurement uncertainty when using the multi-position method

The results of two non-simulation methods, which were published in the article [Sramek, Jankovych 2018], are inserted here for better intelligibility of the article.

Determining the corrected value of the measured object

The developed method regards the true value of a measured object's characteristic (ruby ball diameter) as the average of all measurements of a particular ruby ball's characteristic decreased by the average length measurement error of the used standard E_L by laser interferometer XL 80, and the correction value for the ruby ball diameter measurement E_D. The corrected value of the measured object is calculated by the following relationship [Sladek 2016, Sramek, Jankovych 2018]:

$$y_{corr} = y - E_L - E_D, \tag{1}$$

where:

y is the average value of all measurements of a particular characteristic,

E_D is correction for the ruby ball size measurement,

E_L is average length measurement error obtained with laser interferometer XL80.

It is calculated by the following relationship:

$$E_L = \frac{1}{n_3}\sum_{i=1}^{n_3}\frac{L_{meas std} - L_{calstd}}{L_{calstd}}, \tag{2}$$

where:

n_3 is total number of standard ball measurements with laser interferometer XL80,

L_{calstd} is length of the measured object obtained during its calibration,

$L_{measstd}$ is average length value of the object obtained during its measurement.

Determination of the measurement uncertainty

Definition of the relationship used to calculate the expanded measurement uncertainty in nano-CMM has been made in compliance with generally used practice and described in international documentation [CSN EN ISO 17025:2018, ISO 15530-3:2012, EA 4/02 M: 2013, TNI 01 0115:2009], CMI internal documentation, technical standards and scientific publications [Sladek 2016, Seggelen 2007, Sramek, Jankovych 2018]:

$$U = |E_D| + |E_L| + \\ + k\sqrt{u_{rep}^2 + u_{geo}^2 + u_{corrL}^2 + u_{temp}^2 + u_{prob}^2}, \tag{3}$$

where:

E_D is correction for the measurement of the ruby ball,

E_L is average error of measurement of ruby ball diameter by laser interferometer XL80,

k is expansion coefficient,

u_{rep} is standard measurement uncertainty caused by repeatability of nano-CMM (coverage factor),

u_{geo} is standard measurement uncertainty caused by geometric error of nano-CMM,

u_{corrL} is standard measurement uncertainty of ruby ball diameter by laser interferometer XL80,

u_{temp} is standard measurement uncertainty caused by the impact of temperature during the measurement,

u_{prob} is standard measurement uncertainty caused by touch-robe scanning system Gannen XP.

The above definition was adapted to the general practice and rules of the CMI accredited calibration laboratory. This alteration reflects the chosen measuring method and respects the main sources of the measurement uncertainty that were determined during a large set of measurements. The expanded measurement uncertainty does not include corrections eliminating the systematic error caused by the use of a non-calibrated object. Their impact is reflected in standard deviation, pursuant to European accreditation documents [EA 4/02:2013, Sramek, Jankovych 2018]:

$$U_{mult} = k\sqrt{u_{rep}^2 + u_{geo}^2 + u_{corrL}^2 + u_{temp}^2 + u_{prob}^2 + u_L^2}, \tag{4}$$

where:

u_L is standard measurement uncertainty determining correction for the measurement of a non-calibrated object in nano-CMM.

3.2 Nano-CMM measurement uncertainty when using the substitution method

Definition of the measurement uncertainty calculation

Definition of the relationship for calculation of the expanded measurement uncertainty in nano-CMM is also created in compliance with generally acknowledged practice described in international documents [CSN EN ISO 17025:2005, ISO 15530-3:2004, EA 4/02 M: 2013 and TNI 01 0115:2009] and latest scientific publications [Sladek 2016, Seggelen 2007, Sramek, Jankovych 2018].

$$U = k\sqrt{u_e^2 + u_p^2 + u_w^2 + u_b^2}, \tag{5}$$

where:

k is expansion coefficient (coverage factor),

u_e is standard measurement uncertainty caused by the used standard,

u_p is standard measurement uncertainty evaluated by the A method (see EA 4/02 M),

u_w is standard measurement uncertainty caused by accidental material changes of the measured object and by influences during its manufacturing, it also depends on the measurement strategy,

u_b is standard measurement uncertainty associated with determination of the systematic measurement error of the standard's dimension.

The given definition was closely specified based on experience with measurements and standard practice and rules of the CMI Brno accredited calibration laboratory. This modification reflects the chosen measurement method and main sources of the measurement uncertainty that have been identified and analyzed during a large set of measurements:

- Resolution of the measuring system nano-CMM;
- Impact of the Gannen XP probe's touch;
- Standard deviation from repeated measurements;
- Calibration uncertainty of the used standard;
- Uncertainty of knowledge of thermal expansion of the measured object;
- Uncertainty of knowledge of thermal expansion of the nano-CMM body material;
- Calibration uncertainty of the used thermometer;
- Measurement uncertainty of the real temperature of the nano-CMM working area;
- Impact of cleaning of the measured object;
- Impact of fixing of the used standard.

Based on this analysis, the better specified formula for calculation of the expanded measurement uncertainty by the substitution method is as follows [Sramek, Jankovych 2018]:

$$U_{subs} = k\sqrt{u_r^2 + u_{prob}^2 + u_a^2 + u_e^2 + u_{temp}^2 + u_{cl}^2}, \tag{6}$$

where:

u_r is standard measurement uncertainty caused by the impact of the nano-CMM resolution,

u_{prob} is standard measurement uncertainty caused by probe Gannen XP,

u_a is standard measurement uncertainty evaluated by the A method,

u_e is standard measurement uncertainty caused by the used standard,

u_{cl} is standard measurement uncertainty caused by the impact of impurity of the measured object,

u_{temp} is standard measurement uncertainty caused by the impact of temperature on the measurement.

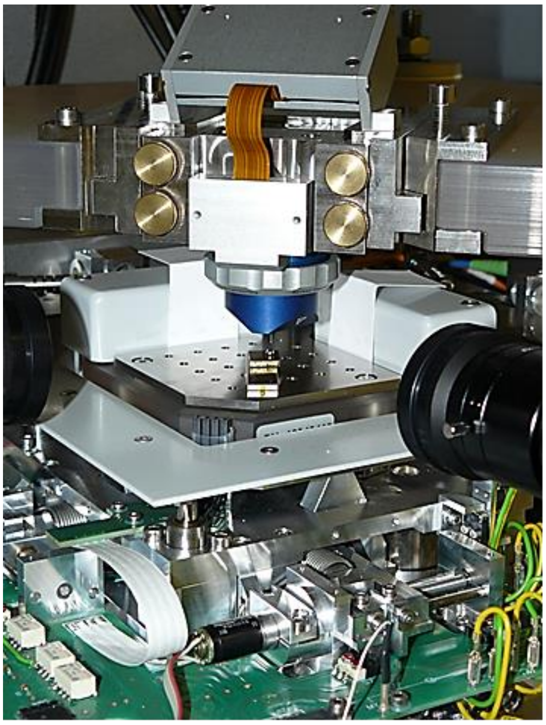

Figure 4. The working area of the measuring instrument nano-CMM

3.3 Nano-CMM measurement uncertainty when using the Monte Carlo method

Definition of the measurement uncertainty calculation

The simulation of the experimental measurement, or the determination of the measurement uncertainty, was performed after refinement and definitive definition of the mathematical model, which optimally described the measurements on nano-CMM using the Gannen XP nano-probe. The simulation itself was carried out in collaboration with colleagues from the Primary Pressure Standardization Department of CMI using the MatLab® software environment.

The MCM method does not only include one value - for example, the average of the measurements, but it examines the behavior of the system for different values of the probability distribution of the input variables. These values oscillate near the average value of the measured quantity, so the equation describing the nano-CMM mathematical model can be compiled as described in chapters 3.1 and 3.2.

A random number generation system based on a specific probability distribution of the input functions can be successfully used for the model described above. Sampling is based on a number generator of rectangular probability distribution. After generating a number (or several numbers) of a rectangular distribution R (0,1), it is possible, using appropriate transformations, to accept a randomly selected number into the model of any other probability distribution type [Sladek 2016, Pernikar 2015].

The transformation procedure is described in detail in Appendix GUM [TNI 01 4109-3.1:2011]. For the rectangular distribution, Wichmann-Hill Random Number Generator was selected, which passed the "accuracy" test and is also used to validate the effect of pseudo-random number generators. The probability number P = 0.95 was chosen as the number of experiments M = 10^6, which is sufficient for the correct determination of the probability distribution of the output variable by the Monte Carlo method [Sladek 2016].

After running the iterations the number of iterations M for all distributions, the numbers were inserted into the mathematical model. In this way, the number of M values of the measured (input) quantity was reached, which, on the other hand, after the respective transformations, represents the probability distribution of the output variables. Based on this model (function), it was possible to determine the desired parameters of the output variable - the expected standard uncertainty value [Sladek 2016].

One of the basic elements of this method is the determination of the mathematical model describing the nano-CMM measuring system.

Mathematical model for Monte Carlo method

For the description of the real mathematical model, the relation (1) was used as the basis for the measurement error of the monitored system. The general formula for expressing the value of the measured (corrected) y_{cor} is:

$$y_{cor} = \bar{y} - \Delta_S \quad , \tag{7}$$

where:

$\bar{y}$ is the arithmetic mean of nano-CMM NNM-1 indications of y in a given measurement cycle, Δ_S is the systematic error of nano-CMM NNM-1.

Mathematical model of measurement for the multi-position method

The mathematical model of measurement on the nano-CMM instrument can be described as a function that serves to determine the corrected value of the y_{cor} output variable and can be described by a relationship based on the latest scientific publications [Sladek 2016, Seggelen 2007] and normative documents [ISO 15530-3:2012, CSN EN ISO 10360-3:2010]:

$$y_{cor} = \bar{y}(1+\alpha_N \Delta t) - L\frac{1}{3n}\sum_{j}^{3}\sum_{i=1}^{n}\frac{L_{meastd}(1+\alpha_W \Delta t) - L_{calstd}}{L_{calstd}} - \frac{1}{n_4}\sum_{i=1}^{n_4}(D_{meas} - D_{cal}) \quad , \tag{8}$$

The corresponding modification of this equation for the multi-position method is a mathematical model of measurement involving the expression of E_L and E_D values from (3), which is expressed as:

$$y_{corm} = \bar{y}(1+\alpha_N \Delta t) - L\frac{L_{meastd}(1+\alpha_W \Delta t) - L_{calstd}}{L_{calstd}} \quad , \tag{9}$$

where:

y_{corm} is the corrected measurement result for the multi-position method,

$\bar{y}$ is the average of all measurements of a given object characteristic,

Δt is the deviation of the temperature of the nano-CMM body and balls when measured from 20 ° C,

α_W is the coefficient of extensibility of the ruby ball material,

α_N is the coefficient of extensibility of the body material of nano-CMM,

L is the measured length in meters,

$L_{measstd}$ is the result of length measurement,

L_{calstd} is the calibration value of the length standard,

D_{meas} is the result of measuring the internal dimension of the length standard,

D_{cal} is the calibration value of the internal dimension of the length standard.

For the equation (9) and for the mathematical measurement model, a random number generator generated 10^6 numbers using

Matlab®. The script for determining the measurement uncertainty using the Monte Carlo method was already described in chapter 3.1. As with the substitution method, the Grubbs test of outliers from a set of measured data was first performed. The input data was the same as used for the non-simulative method in chapter 3.2. Thus, the Grubbs test was not repeated. The resulting histogram and the results of simulation of the ruby ball measurement by *d* = 1 mm by the Monte Carlo method for the multi-position method are given in Table 1 and Figure 6.

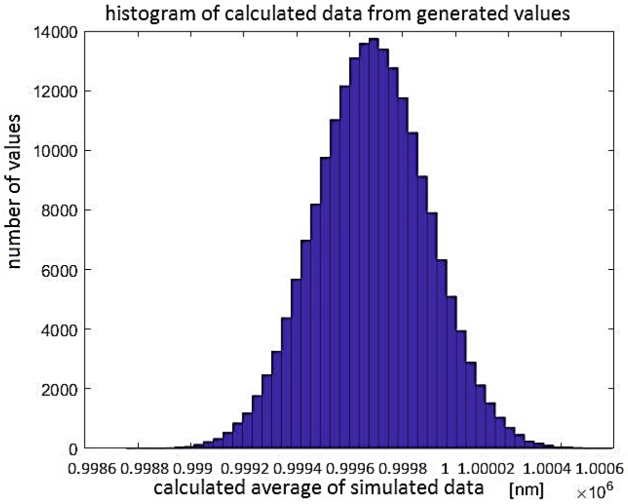

Figure 6. Histogram of calculated data from generated values for ruby ball diameter *d* = 1mm (multi-position method)

Mathematical model of measurement for the substitution method

For the sake of completeness and the possibility of a full-fledged comparison, a mathematical model of the nano-CMM instrument for the substitution method of measurement uncertainty was created. This relationship is again based on the latest scientific publications [Sladek 2016, Seggelen 2007] and normative documents [ISO 15530-3:2012, CSN EN ISO 10360-3:2010]:

$$y_{cors} = \bar{y}(1+\alpha_W \Delta t) - (y_w - x_{cw}) , \qquad (10)$$

where:

y_{cors} is the corrected measurement result for the substitution method,

$\bar{y}$ is the average of all measurements of a given object characteristic,

α_W is the coefficient of linear expansion of the material of the object being measured,

Δt is the deviation of the measured object temperature from 20 ° C,

y_w is the average of all standards measurements (using nano-CMM),

x_{cw} is the value of the standard specified in the calibration protocol.

For the above relationship (10) and for the calculation of the expanded measurement uncertainty, the random number generator 10^6 was generated using the Matlab® program as well as for the previous method. The next procedure was the same as in this chapter for the multi-position method. The resulting histogram and the results of simulation of the measurement of the ruby ball by *d* = 1 mm by the Monte Carlo method for the substitution method are given in Table 1 and Figure 7.

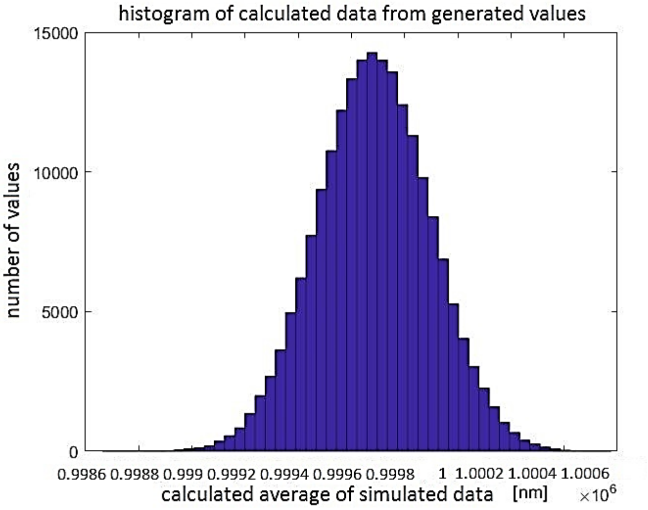

Figure 7. Histogram of calculated data from generated values for ruby ball diameter *d* = 1 mm (substitution method)

4 COMPARISON OF RESULTS OF BOTH METHODS

To determine the measurement accuracy of the nano-CMM NNM-1, the expanded measurement uncertainty was determined by both non-simulation methods for all diameters of ruby balls. This solution provided a full range of measurements of the nano-CMM NNM-1 instrument. In addition, the Monte Carlo measurement uncertainty was chosen. The simulation method makes it possible to replace measured values from experiments. This fact represents a considerable saving of time and has a positive economic effect. Table 1 summarizes the individual measurement uncertainty values determined by various methods for all diameters of the ruby sphere (1-4mm) that represent all evaluation methods. The color indication of the individual contributions of the measurement uncertainty is identical to the figures 8 and 9 for better clarity.

Expanded uncertain.	*d* = 1mm	*d* = 2mm	*d* = 3mm	*d* = 4mm
U_{subst}	57.4	57.5	57.7	57.9
U_{mult}	78.1	53.2	55.2	54.3
$U_{substMC}$	55.8	51.8	53.6	53.0
U_{multMC}	75.6	55.6	55.9	56.2

Table 1. Comparison of expanded measurement uncertainty values for all methods [*nm*]

Figure 8 shows column diagram of the obtained results. The expanded measurement uncertainty values correspond to the non-simulation and simulation methods used.

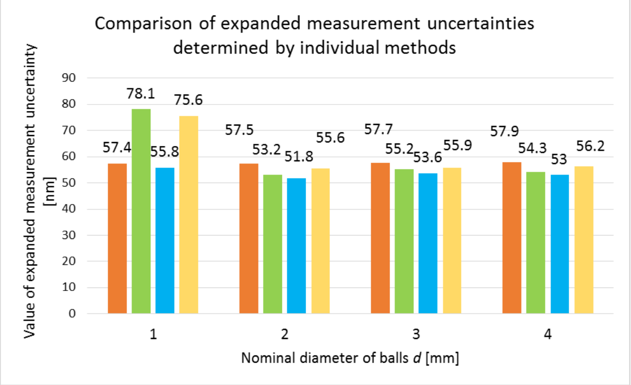

Figure 8. Values of the expanded measurement uncertainty determined by the substitution and multi-position methods [*nm*]

Figure 9 shows a line diagram of the obtained results for all ruby ball diameters (1-4mm).

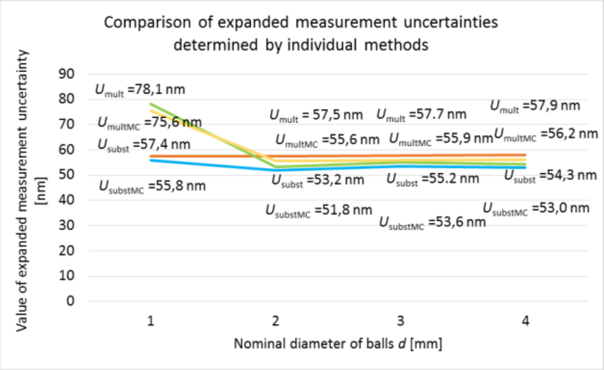

Figure 9. Line diagram of expanded measurement uncertainty of ruby balls with nominal diameters *d* = (1-4) mm.

Expanded measurement uncertainty of the ruby ball diameter *d* = 1 mm determined by the multi-position method is U_{mult} = 78.1 nm after rounding. Expanded measurement uncertainty of the ruby ball diameter *d* = 1mm determined by the substitution method is U_{subs} = 57.4 nm after rounding. Expanded measurement uncertainty of the ruby ball diameter *d* = 1 mm determined by the Monte Carlo method (multi-position version): U_{multMC} = 55.8 nm after rounding. Expanded measurement uncertainty of the ruby ball diameter *d* = 1 mm determined by Monte Carlo method (multi-position version) is U_{subsMC} = 55.8 nm after rounding. The increased value of expanded uncertainty for the ruby ball with *d* = 1 mm is due to the diameter d_{saf} = 0.12 mm of the touch probe Gannen XP. A further reduction in uncertainty can be achieved by using a smaller diameter touch probe.

5 DISCUSSION

This paper briefly dealt with the current situation in the field of determining the accuracy of measurements in nanometrology using the nano-CMM, which is located in the laboratory of the primary nanometrology and technical length department of CMI. This precision CMM is a higher standard of metrology instruments, especially composed by classic multi-axis and multi-purpose measuring instruments that, thanks to their functional principle and design, cannot provide measurements as accurate as nanotechnologies.

The paper presents an original calculation procedure, which replaces the simplified method of measuring uncertainty specified by the instrument manufacturer. The solution includes a detailed description of the measurement uncertainty of nano-CMM using two non-simulation methods and Monte Carlo simulation. A prerequisite for this result was making of a comprehensive set of measurements, which was associated with the development of suitable measurement methods and measuring hardware.

The paper also presents a comparison of the results of all three measurement uncertainty methods used to quantify the measurement accuracy of nano-CMM.

Such a comprehensive and detailed solution for nanometrology has never before been implemented in the Czech Republic or in other EU countries.

6 CONCLUSIONS

The evaluation of large sets of measured data shows that all used methods (simulative and non-simulative) allow for a sufficiently accurate determination of the measurement accuracy in nanometrology.

The nano-CMM is an important element in the field of primary nanometrology within the system of metrological traceability, especially in the calibration laboratory of the Czech Metrology Institute in Brno. However, due to the scale and characteristics of individual factors affecting measurement uncertainty, this field is so complex that this article cannot describe all aspects of the nano-CMM instrument used as an accurate measurement standard.

The presented measurement uncertainty values show a reduction in the accuracy when measuring length of 1mm or less. In this case, the choice of touch sensor with a smaller sapphire ball diameter is appropriate.

The authors are currently working on an accredited calibration procedure for measurement on the nano-CMM according to the Czech Accreditation Institute using all three methods described.

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