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Variability in measurements of micro lengths with a white light interferometer

Carlo Ferri and Emmanuel Brousseau

Manufacturing Engineering Centre, Cardiff University

Newport Road, Cardiff, CF24 3AA, United Kingdom

telephone: 0044 (0) 7985744969

email: ferric@cardiff.ac.uk

Abstract

The effect of the discretionary set-up parameters scan length and initial scanner position on the measurements of length performed with a white light interferometer microscope was investigated. In both analyses, two reference materials of nominal lengths 40 and 200 μm were considered. Random effects and mixed effects models were fitted to the data from two separate experiments. Punctual and interval estimates of variance components were provided.

KEY WORDS: Random effects ANOVA, linear mixed models, white light interferometry, WLI, uncertainty, gauge capability analysis.

1 Introduction

Metrology has been recognised as one of the key enabling technologies to support the current efforts in micro and nano manufacturing [1]. White light interferometer (WLI) microscopy is one of the measurement methods giving this support. In fact, it provides measurements of surface roughness and heights at both micro and nano scale. In particular, WLI microscopes use a charge-coupled device (CCD) camera to record the

intensity of bright and dark fringes for each pixel in the field of view while the object under observation is scanned perpendicularly to its illuminated surface with a vertical movement of the interferometric objective (scanner element). The extension of this vertical movement is called scan length. Then, by applying built-in algorithms to the recorded intensities, the topography of the inspected surface is constructed.

For the particular microscope under investigation, it is argued from the manufacturer manuals ([2], [3]), that two degrees of freedom are left to the operator in setting up the instrument for a measurement task. In fact, the scan length and the initial position of the scanner element can be selected in an infinite number of manners while complying with the prescriptions of the manuals. For this reason, these two parameters were experimentally investigated in order to assess their contributions to the uncertainty of the measurement results [4].

In these experiments, two purpose built measurands were employed as reference materials [5]. A procedure was in fact developed to establish step heights in the micro range by using certified gauge blocks of grade 1 [6] traceable in accordance with BS 4311-3 [7]. Two gauge blocks were used in preparing each step height. They were wrung side by side onto a quartz optical parallel. The use of the transparent optical parallel allowed the quality of the wringing procedure to be assessed by observing the presence of interference colour fringes and bright spots on the two wrung faces [8].

In the next section the contribution to the variability of the measurements results due to the scan length is estimated, whereas the contribution due to the initial scanner position is estimated in the subsequent section. Conclusions are drawn thereafter.

2 Scan length

2.1 Experimental set-up

The nominal lengths of the two selected reference materials, henceforth also referred to as step heights, were 40 and 200 μm . For a given scan length, each of them was measured eight times. In total, five different scan lengths were selected to exceed each nominal length by 10%, 15%, 20%, 25% or 30%. These five values are a sample drawn from the infinite population of scan lengths that conform with the specifications provided in the instrument user manuals ([2], [3]), namely the interval $I = [10\%, 30\%]$.

The overall number of measurements for each reference material was equal to forty.

While performing the tests, the initial position of the scanner was set inside the admissible range prescribed in the manuals ([2] , [3]), without following any specific experimental strategy. The contribution to the overall variability of the test results due to an unspecified scanner initial position is in fact not expected to affect significantly the estimate of the variability in the measurement results accounted for by the scan length. The unspecified initial scanner position is instead expected to increase the variability of the error term in the model fitted to the data.

All the other hardware and software set-up parameters of the measuring system were kept constant during the experiment. The sequence of the measurements on each reference material was randomly selected from 40! permutations. Moreover, all the results were obtained from the same location on a reference material and without re-positioning the stage to a pre-specified origin between the measurements.

2.2 Results

Let h_{ijk} be the k -th measurement result ($k = 1, \dots, 8$) obtained using the j -th level of scan length ($j = 1, \dots, 5$) on the i -th reference material with $h_{nom,i}$ step height ($i = 1, 2$). Let s_{ijk} be the percentage deviation of the i -th step height from h_{ijk} , namely: $s_{ijk} = (h_{nom,i} - h_{ijk}) / h_{nom,i}$.

The notched box plot of Figure 1 (cf. [9]) shows only positive values of s_{ijk} due to the fact that the experimental set-up investigated is not the end effect of a calibration procedure (cf. [10]). In fact, while estimating the variability of a measurement system, its bias ‘will have no influence and can be ignored’(section 5.1.1.2 in [11]). This assumption holds unless there is a significant interaction between the bias and the spread of the measurement results. The physical design of the measuring system investigated does not however appear to justify such an interaction. Therefore, no calibration is performed in this study. Moreover, it appeared reasonable to assume that the calibration state was the same throughout the whole experimental activity. Such an assumption hinges on the reasonably stable environmental conditions of the laboratory and the short time needed to carry out all the tests (some hours).

Figure 1 also displays that the medians of several pairs of groups are significantly different. In fact, the width of the notches represents a 95% Gaussian-based asymptotic

confidence interval for the median calculated as described in [9] (cf. equation 7.3, ib.). Therefore, if the notches about two medians do not overlap, these two medians are significantly different approximately at 95% significance level. This is for instance the case of the pairs (10%,15%), (10%,20%), (20%,30%) for the step height 40 μm and (10%,25%), (20%,30%) for the step height 200 μm . In addition, a descending pattern while increasing the scan length is also apparent in Figure 1. On the basis of this analysis of the experimental evidence it can be concluded that changing the scan length does induce a significant bias on the measurement results.

No extreme data outlying from the majority of the measurement results grouped by scan length level is present in Figure 1. Moreover, the distribution of the s_{ijk} appears approximately symmetric around the median. It can also be noticed that the spread of the results does not show major differences for different scan lengths.

[Figure 1 about here.]

A random effects ANOVA model was fitted to the data in order to estimate the contribution to the overall variability of the measurements results that is accounted for by the scan length. h_{ijk} was selected as response variable, $h_{nom,i}$ and $t_{s,j}$ as the unobservable random effects due to the random draw of the two reference materials and the five scan lengths from their respective populations. Namely, it holds:

$$h_{ijk} = \mu_s + h_{nom,i} + t_{s,j} + e_{ijk} \quad i = 1, 2 \quad j = 1, \dots, 5 \quad k = 1, \dots, 8 \quad (1)$$

where μ_s is the overall mean, $h_{nom,i}$'s and $t_{s,j}$'s are assumed to be normally independent and identically distributed (NIID) random variables with mean zero and constant variances σ_h^2 and σ_t^2 , respectively, i.e. $\{h_{nom,i}\} \sim NIID(0, \sigma_h^2)$ and $\{t_{s,j}\} \sim NIID(0, \sigma_t^2)$. The e_{ijk} is the random error of the k -th measurement result obtained on the i -th reference material using the j -th scan length. It arises from all the sources of variability of the measurement results of the i -th reference that are not due to the scan length. It is also assumed that $\{e_{ijk}\} \sim NIID(0, \sigma^2)$.

Moreover, by assuming that $h_{nom,i}$'s, $t_{s,j}$'s and e_{ijk} 's are all between themselves independent, the variance of the generic h_{ijk} is then given by

$$V(h_{ijk}) = \sigma_h^2 + \sigma_t^2 + \sigma^2 \quad (2)$$

where σ_h^2 , σ_t^2 and σ^2 are called variance components.

The parameters of the model, namely μ , σ_h , σ_t and σ , were estimated using the restricted (or residuals) maximum likelihood (REML) method as it is implemented in the `lme` function from the `nLme` library for R [12]. This library is documented by its main authors in [13]. The formulation of the model is displayed in Table 1, whereas the estimates obtained are shown in Table 2 (model I). The number of digits for the estimates in that table is consistent with the resolution of the measuring system in the vertical direction (2.2 nm according to [3]).

[Table 1 about here.]

[Table 2 about here.]

The realisations of the residuals \hat{e}_{ijk} of this model, standardised using $\hat{\sigma}$ and displayed in Figure 2, exhibit however a mild pattern against the run order of the measurement results. To confirm such a qualitative observation two separate linear models of the residuals, standardised using $\hat{\sigma}$, were fitted against the sequence order, namely $\hat{e}_q = \beta_0 + \beta_1 \cdot x_q + e_{new,q}$ with $q = 1, \dots, 40$, one for each reference material. The estimation of β_0 and β_1 was performed using the `lmList` function of the library `nLme` [13]. The obtained estimates $(\hat{\beta}_0, \hat{\beta}_1)$ were $(-0.6266, 0.03056)$ and $(-3.409, 0.05634)$ for the 40 and 200 μm step height, respectively. Subsequently, after graphically assessing the assumption of normality of the $e_{new,q}$'s in a normality plot, a 95% confidence interval was calculated for the β_0 's and the β_1 's for the two reference materials, i.e. $\hat{\beta}_l \pm t_{0.975,38} \cdot \hat{\sigma}(\hat{\beta}_l)$ where $l = 0, 1$ and $t_{0.975,38}$ is the 97.5% quantile of the Student's t distribution (c.f. for instance [14]). This produced the intervals $(-1.067, -0.1858)$ and $(-5.046, -1.771)$ for the two β_0 's, $(0.01183, 0.04930)$ and $(0.02976, 0.08292)$ for the two β_1 's.

[Figure 2 about here.]

From this numerical evidence two conclusions are drawn. First, the effect of the test sequence on the results is significant. In fact both the confidence intervals for β_1 's do not contain the origin. Second, the confidence intervals for the β_1 's have an overlap, whereas those for the β_0 's have not. It is therefore argued that the effect of the nominal length on the measurements results is significantly affecting only the intercepts but not

the slope of the relationship between the measurement results and the sequence of the tests.

As a consequence of these observations, a second model was fitted to the data where the dependence of the measurement results on the test sequence was introduced. In this second model, the random effect due to the grouping factor step height is considered as affecting only the intercept of the model but not the rate of changing of the measurements over the time (slope). This linear mixed effects model is formally described as follows:

$$h_{ijk} = \mu_s + \beta \cdot x_{ijk} + h_{nom,i} + t_{s,j} + e_{ijk} \quad i = 1, 2 \quad j = 1, \dots, 5 \quad k = 1, \dots, 8 \quad (3)$$

where $x_{ijk} = 1, \dots, 80$ is the order in the sequence of tests and the symbol β indicates a parameter to be estimated. The assumptions underlying equation 1 also hold in equation 3, therefore equation 2 is still valid for equation 3. The parameters of the models were estimated with the REML method using the function `lme` in a similar way as for equation 1. The estimates are shown in Table 2 (model II). From equation 2, therefore, it follows that $\hat{V}(h_{ijk}) = 12003.990 \mu m^2$.

Given a pre-specified step height in the range of the two values tested (40 and 200 μm), the selection of the scan length in the range of the admissible values accounts for about 60.84% (i.e. $100 \cdot 0.312^2 / (12003.990 - 109.562^2)$) of the variance of a series of test measurements performed in quasi-repeatable conditions. The prefix quasi denotes that the initial position of the scanner element was not kept constant, but selected in a random fashion inside the admissible range as a generic operator would do after reading the user manual. Approximate 95% confidence intervals for the parameters of the model were obtained using the approximate asymptotically normal distributions of the REML estimates (cf. section 2.3 and 2.4.3 in [13]) so as it was implemented in the function `intervals` of the library `nlme`. Of particular interest in this study are the 95% confidence intervals $0.152 \mu m < \sigma_t \leq 0.640 \mu m$ and $0.204 \mu m < \sigma \leq 0.283 \mu m$. Thus, while varying the scan length complying with the prescriptions of the instrument manuals ([2], [3]), the measurement results are different at about 95% significant level. In fact, the approximate 95% confidence interval for σ_t has a strictly positive infimum.

The realisation of the residuals from the model of equation 3 did not display any violation of the assumed independence of the errors. In particular, when plotting them

against the run order, the pattern previously observed in Figure 2 for the realised residuals of the first model (equation 1) was not present anymore. Also a normality plot of the realisation of the residuals did not display any denial of the assumed normality of the errors. A graphical analysis of the realised residuals versus the fitted values did not show any departure from the hypothesis of equal variance of the errors.

3 Scanner initial position

3.1 Experimental Set-up

Two different initial positions of the scanner were considered, each of them allowing some fringes to be observable. The first position was selected at the highest point of the scanner for which fringes were still visible (TOP). The second position was selected at the middle of the range between the highest and the lowest points for which fringes were visible (MID). The step heights were the same as in the previous section, namely 40 and 200 μm . The scan length was kept at the constant level of 30% in excess of the step heights throughout the whole experiment, that is 52 and 260 μm for the 40 and 200 μm step height, respectively.

In order to hinder the dependence of the measurements results on the sequence of the tests as it appeared in the previous section, each of the four experimental conditions, i.e. (TOP, 40 μm), (MID, 40 μm), (TOP, 200 μm), (MID, 200 μm), were randomly assigned to the run order. Each of the ten replicates of each experimental condition was identified by an integer from 1 to 40. Then one of the 40! permutations was randomly selected to identify the sequence of the tests.

3.2 Results

The results of the experiment are shown in Figure 3, where both the s_{ijk} 's and the h_{ijk} 's are displayed in part (a),(b) and (c), (d), respectively. In this context, the subscript j indexes the initial position of the scanner element ($j = 1, 2$ for TOP and MID respectively), whereas the other indices have the same meaning as in the investigation concerning the scan length, with $i = 1, 2$ and $k = 1, \dots, 10$.

[Figure 3 about here.]

Due to the relative position of the notches in Figure 3, which was obtained with R using the function `boxplot`, it is argued that the initial scanner position is borderline significant in affecting the measurement results for the 40 μm step height but not so for the 200 μm . The distribution of the results around the median appears approximately symmetric, apart from the group MID for the 40 μm step height. Two results appear lying far apart from the majority of the data in the group MID of the 200 μm step height. These two data were second and fourth in the run order. Although no explicit assignable cause was found, it is believed that the occurrence of an unobservable contaminating factor in the early operation of the measuring process is more likely than the two data being generated by the same process that generated the other data. This statement is also supported by the observation of some instability of the measuring process shortly after its start up. Consequently, two analyses of the data were conducted, with and without these two data. The first of these produced a much larger estimate of the variability accounted for by the initial scanner position. However, in the light of the argumentation above, only the analysis with the two outlying data removed is reported in detail.

The interquartile ranges identified by the the lower and higher hinges, i.e. the horizontal line segments of the boxes, in part (a) and (b) of Figure 3, are (0.53%, 0.36%) and (0.19%, 0.22%) for the (TOP, MID) groups of the 40 and 200 μm step height respectively. These two sub-figures with the y-axis in percentage highlight the impact on the spread of the measurements results taken in repeatability conditions due to quantities that may otherwise be underestimated (cf. section 3.14 in [11] for a definition of repeatability conditions). In fact, the same interquartile ranges when expressed in units of lengths, as in part (c) and (d) of Figure 3, amount to (0.21, 0.14) and (0.38, 0.43) μm for the 40 and 200 μm step height respectively. The variability of a series of measurements results taken in repeatability conditions appears to increase with the step height when expressed in unit of length, whereas the same variability appears to decrease when expressed in percentage deviations from the nominal step height. In both cases, when fitting a model for drawing quantitative conclusions about the measuring process from the experimental data, it is expected that some unequal variance of the errors is to be encountered. Similarly to the analysis of the scan length, the following random effect model was first fitted to the data:

$$h_{ijk} = \mu_p + h_{nom,i} + t_{p,j} + e_{ijk} \quad (4)$$

$$i = 1, 2 \quad j = 1, 2 \quad k = 1, \dots, K_i \quad K_1 = 10 \quad K_2 = 8$$

where μ_p is the general mean, the $t_{p,j}$'s are the random effects on the h_{ijk} 's due to the initial scanner position, with $\{t_{p,j}\} \sim NIID(0, \sigma_p^2)$, $\{h_{nom,i}\} \sim NIID(0, \sigma_{hp}^2)$ and $\{e_{ijk}\} \sim NIID(0, \sigma_{pe}^2)$. As before, all these random variables were assumed to be independent all between themselves. The model was fitted to the data in the same way as equation 1 was, using the REML method implemented in the function `lme`. Due to the exclusion of the two outlying cases for the step height 200 μm , the data were unbalanced. However the function `lme` produce sensible REML estimates also with unbalanced data (cf. section 1.3.2 in [13]). The estimates of the parameters are displayed in Table 2 (model III). Among them, $\hat{\sigma}_p$ appears negligible.

The realisation of the residuals standardised by $\hat{\sigma}_{pe}$ and grouped by step height are shown in Figure 4.

[Figure 4 about here.]

In this figure, no effect of the test sequence on the realised residuals is visible. The full randomisation in the assignment of the tests to the run order may have played a part in counteracting this effect that was detected in the previous investigation (Figure 2). Moreover, as expected from the exploratory analysis of Figure 3, the variability of the realised residuals appears to increase, when increasing the step height from 40 to 200 μm .

This variance dependence is even more evident in the box plot of Figure 5, where the same residuals are grouped by step height and initial scanner position. It is also noticed that the deviation of the medians of the groups from zero may raise some concern. These deviations can be due to random fluctuations of the realisation of the residuals around their expected value that is zero. But they can also be due to some unidentified lurking source of variability that should be included in the model. No experimental evidence was however found supporting this second possibility.

[Figure 5 about here.]

The uneven spread of the residuals highlighted in Figure 4 and 5 is incompatible with the assumed equal variance of the errors. Consequently, a second model was fitted to the data where the errors were modelled as having different variances in the two groups

of measurement results identified by the factor step height, namely:

$$\sigma_{pe,m}^2 = \sigma_{new}^2 \cdot \delta_m^2 \quad m = 40 \mu m, 200 \mu m \quad (5)$$

where $\sigma_{new} > 0$ and the unconstrained parameter $\delta_{200 \mu m}$ are to be fitted to the data using the REML optimisation method. Instead, $\delta_{40 \mu m}$ is set to be equal to one. The fitting was accomplished by using the function `lme` with one of the classes `varFunc` of the `nlme` library for specifying variance models of the within-group errors (cf. section 5.2 in [13]). Among these, the class `varIdent` was selected due to the fact that in this study the step height was represented as a random factor and not as a numerical variable.

The two competing models fitting the data were assessed using the likelihood ratio test (LRT) as it is implemented in the function `anova.lme` of the library `nlme` (cf. section 5.2.2 in [13] for its usage in similar cases). The test resulted in $P_{value} = 1.84\%$. This led to reject the null hypothesis that the simpler model (the first) is as adequate as the second in describing the data. The model with variance of the errors depending from the level of step height is therefore to be adopted.

The REML estimates obtained in this model are displayed in Table 2 (model IV). Therefore, from equation 5 it follows that $\hat{\sigma}_{pe,40 \mu m} = 0.126 \mu m$ and $\hat{\sigma}_{pe,200 \mu m} = 0.252 \mu m$.

In a similar manner as in equation 2, given the 40 and 200 μm step heights, from equation 4 and 5 under the specified assumption of independence it is derived that $\hat{V}(h_{1jk}) = \hat{\sigma}_p^2 + \hat{\sigma}_{pe,40 \mu m}^2$ and $\hat{V}(h_{2jk}) = \hat{\sigma}_p^2 + \hat{\sigma}_{pe,200 \mu m}^2$. It hence follows that $\hat{V}(h_{1jk}) = 0.023 \mu m^2$ and $\hat{V}(h_{2jk}) = 0.071 \mu m^2$. Therefore, given the two reference materials, the selection of the initial scanner position in the range of the admissible values accounts for about 31.4% and 10.2% of the overall variance of a series of test measurements performed in repeatability conditions for the 40 and 200 μm step height, respectively. These figures support the common perception that degrees of freedom left to the operator while configuring set-up parameters are increasingly problematic when reducing the nominal size to be measured.

Approximate 95% confidence intervals for the parameters of the model were obtained similarly as in the study of the scan length effect. Of interest in this study are the 95% confidence intervals $0.0157 \mu m < \sigma_p \leq 0.459 \mu m$ and $0.088 \mu m < \sigma_{new} \leq 0.178 \mu m$. The first interval has an infimum greater than zero. Therefore the initial

scanner position set according to the equipment user manuals ([2] , [3]) has a significant effect on the measurement results. The upper bound of this interval is about twenty nine times its lower bound. This large amplitude hence suggests that the precision of the estimate can be substantially improved. The second interval provides an approximate 95% confidence region of the repeatability standard deviation of the process when measuring a 40 μm step height. Such a repeatability standard deviation constitutes a best case scenario. In fact, its other punctual estimate is obtained as $\hat{\sigma}_{new} \cdot \hat{\delta}_{200\mu\text{m}}$, with $1.187 < \delta_{200\mu\text{m}} \leq 3.379$ at an approximate confidence level of 95%.

As in the case of the scan length investigation, an exploratory data analysis of the realisation of the standardised residuals of the fitted model did not exhibit major violation of the assumed independence of the errors and of their variance model that was adopted. Moreover, a normality plot of the realised residuals did not show significant departures from the assumed normality of the errors, even when the residuals were grouped by step height, by initial scanner position and by every distinct combination of step height and initial scanner position.

4 Conclusions

This study has ascertained that the discretionary setup parameters scan length and initial scanner position have a significant effect on the measurement of lengths taken by a WLI microscope in the micrometre range. These findings were supported respectively by a mixed effects model and by a random effect model with variance of the errors depending on the size of the part.

When measuring parts in the micrometre range represented by the two steps of nominal height 40 and 200 μm , the contribution to the variability of the results accounted for by the scan length was equal to a standard deviation ranging in the interval (0.152, 0.640] μm with approximated significance level of 95%. The punctual estimate of this standard deviation was 0.312 μm .

In the experiment leading to these estimates, a dependence of the measurements results on the run order was detected and quantitatively estimated, resulting in an expected 0.015 μm increment in the measurements every next test.

The contribution to the variability of the results from a subsequent separate exper-

iment attributable to the initial scanner position was estimated by a standard deviation spreading across the interval (0.0157, 0.459] μm with 95% approximate significance level. The punctual estimate was 0.085 μm .

In this second experiment the repeatability standard deviation, i.e. the standard deviation of the errors in the fitted model, appeared to be depended on the size of the part. Its smallest value, estimated on the 40 μm step height, was 0.126 μm , spanning the interval (0.088 , 0.178] μm with 95% approximate confidence level.

This study shows practitioners the benefits of finding out the detrimental and often underestimated effects that lurking degrees of freedom in set-up operations may have on the variability of a measuring process.

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Authors' Biographies

Carlo Ferri received a Ph.D. in Micro Manufacturing from Cardiff University (United Kingdom) and a Laurea Degree in Industrial Engineering from the Politecnico di Milano (Italy). He is a member of ENBIS (European Network for Business and Industrial Statistics). His current research interests lie within the scope of this affiliation and within the area of micro-nano manufacturing.

Dr Emmanuel Brousseau obtained his PhD in the Manufacturing Engineering Centre (MEC) at Cardiff University, UK, in the field of automatic feature recognition from 3D Computer-Aided Design models. His overall research interest lies in the field of advanced manufacturing technologies. Currently, he is carrying out post-doctoral research

at the MEC in micro-manufacturing. Dr Brousseau investigates metrology techniques for dimensional measurements and surface characterisation of micro-components.

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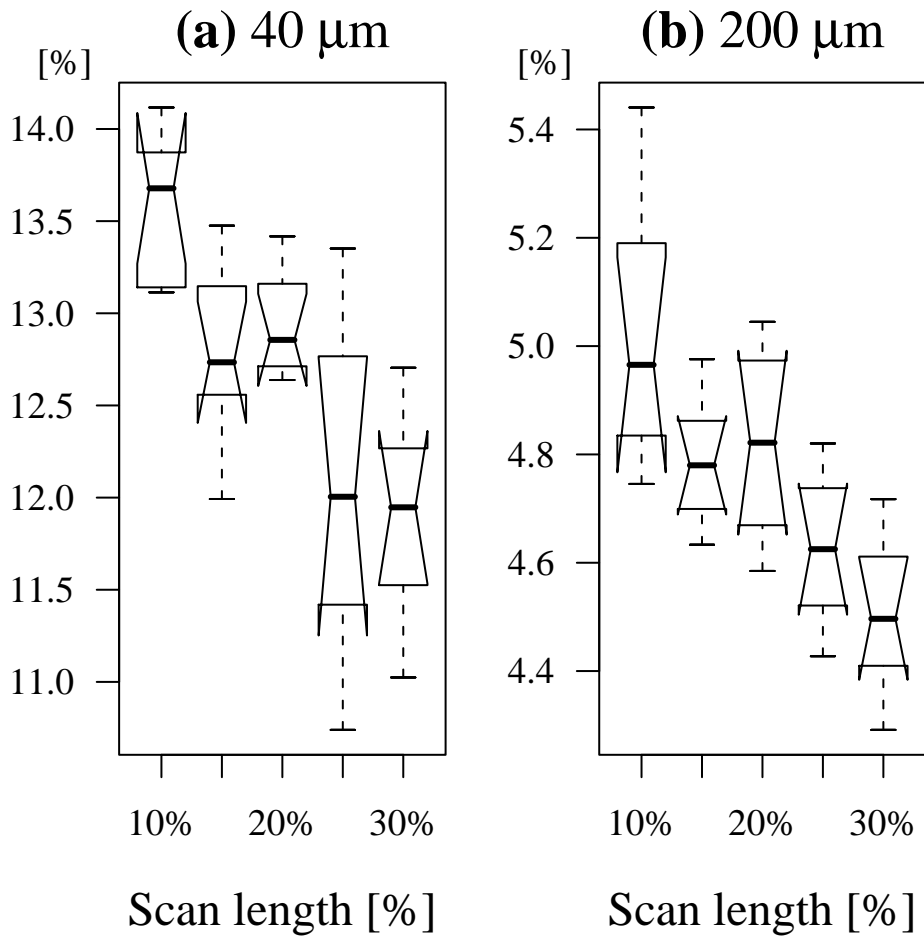


Figure 1: Box plot of the percentage deviations versus percentage scan length for step height 40 and 200 μm .

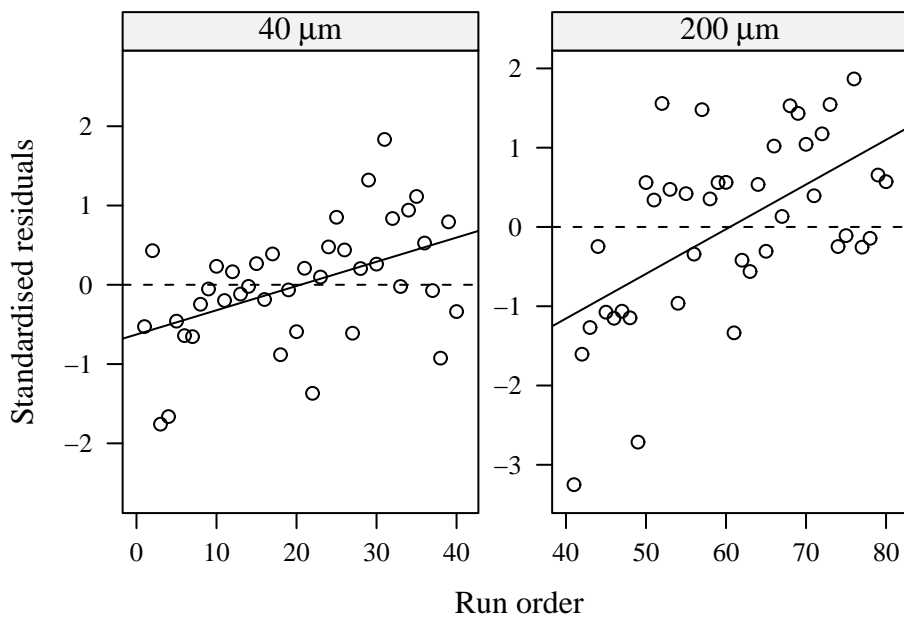


Figure 2: Standardised realisations of the residuals of the model in equation 2 versus the sequence of the tests.

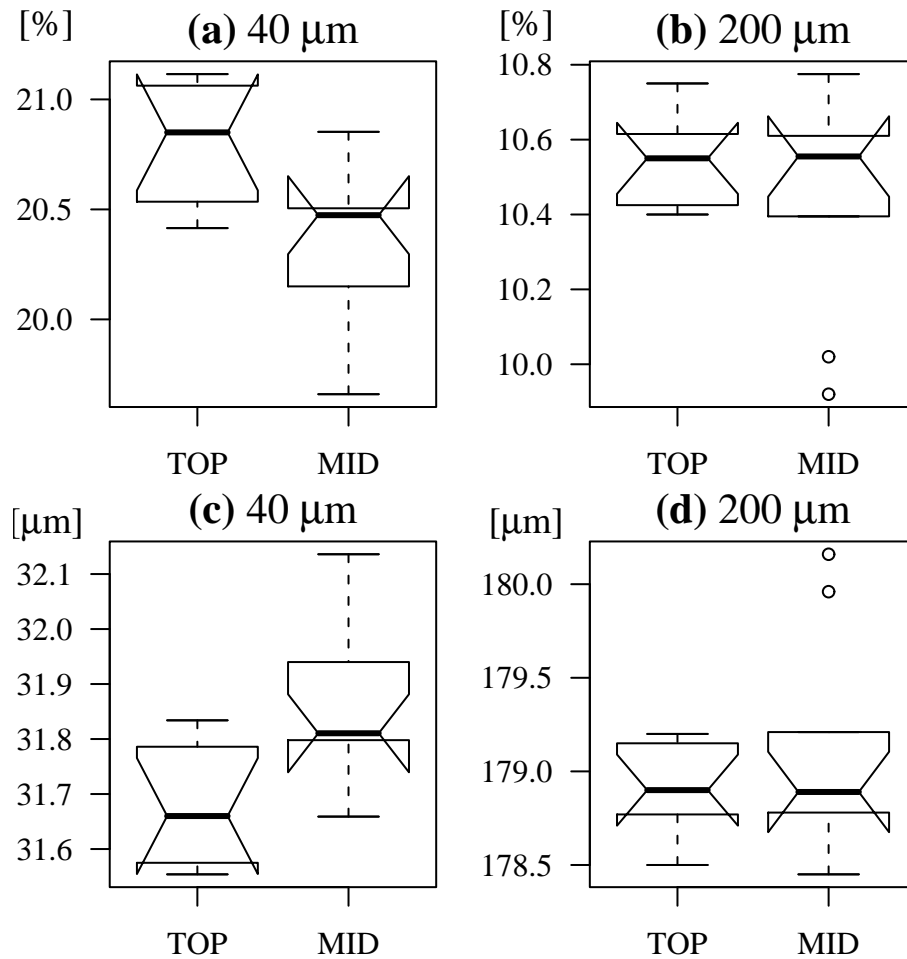


Figure 3: Initial scanner position: notched box plot of the results as percentage deviations from the nominal (s_{ijk} , parts (a) and (b)) and as raw values (h_{ijk} , parts (c) and (d)).

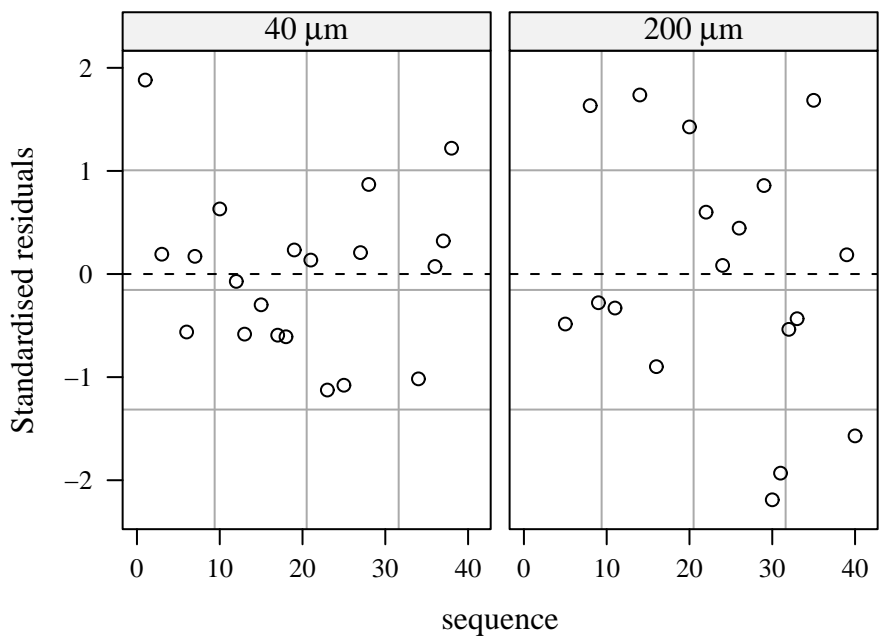


Figure 4: First model: realisations of the standardised residuals against the test sequence when grouped by the step height.

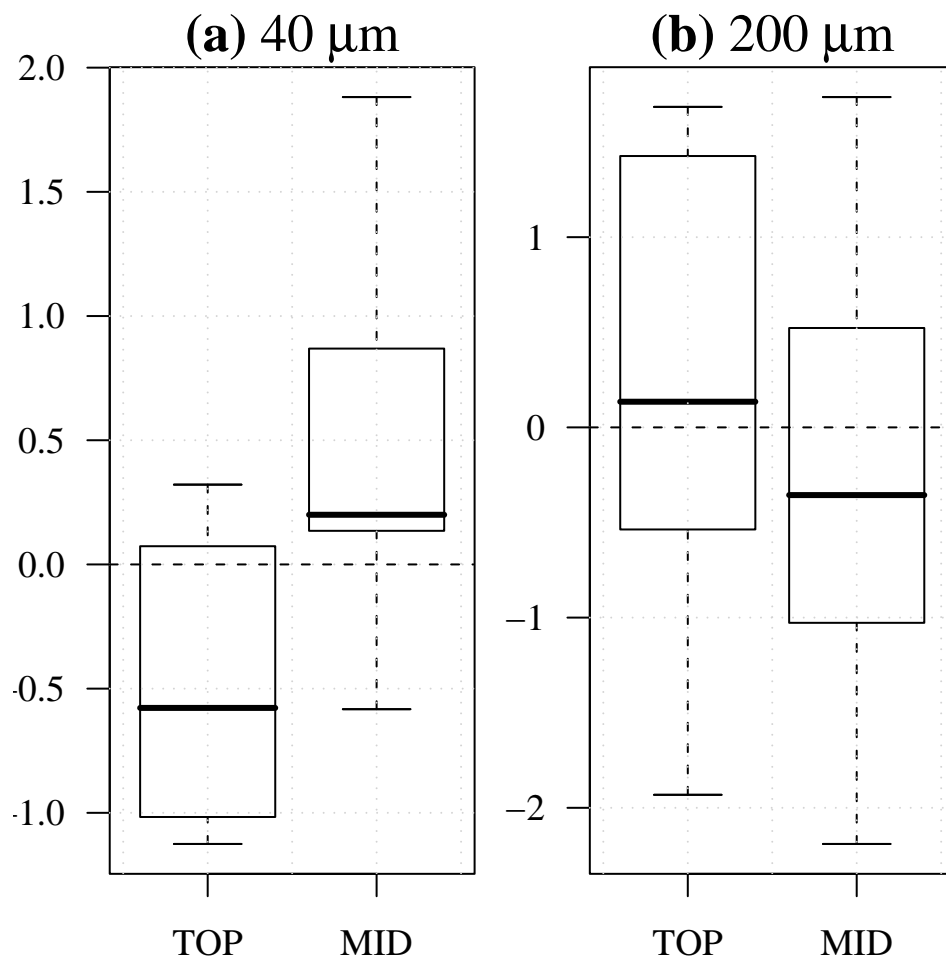


Figure 5: Box plot of the realisations of the standardised residuals grouped by step height and initial scanner position.

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```
> random.eff.lme <- lme(Results ~ 1,  
+ data=exp.data,  
+ random=list(Dummy.factor=pdBlocked(list(  
+ pdIdent(~ Nominal -1),  
+ pdIdent( ~ Scan -1))))))
```

Table 1: Specification of the model of equation 2 with lme in R.

Scan length		$\hat{\mu}$	$\hat{\beta}$	$\hat{\sigma}_h$	$\hat{\sigma}_t$	$\hat{\sigma}$	
I	μm	112.717	—	109.996	0.324	0.291	
II	μm	112.096	0.015	109.562	0.312	0.240	
Initial position		$\hat{\mu}_p$	$\hat{\sigma}_{hp}$	$\hat{\sigma}_p$	$\hat{\sigma}_{pe}$	$\hat{\sigma}_{new}$	$\hat{\delta}_{200\mu\text{m}}^a$
III	μm	105.323	104.017	$3.965 \cdot 10^{-6}$	0.194	—	—
IV	μm	105.326	104.021	0.085	—	0.126	2.003

^adimensionless

Table 2: Estimates of the model parameters for the scan length and for the initial scanner position.