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Spectral assessment of surface topography

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Abstract

The digital industrialization is revitalizing the way that manufactured products are conceived. The opportunity of several prevailing technologies allows products' digital modelling, and enhanced productivity, with cost-efficient solutions. Even so, corresponding effective metrology methods are urgently needed to preserve the manufacturing digitalization whole perspective.

In this background, an alternative assessment of optical surface topography measurements was demonstrated on micrographs' spatial frequency content. Specifically, the power spectral density (PSD) was used for the evaluation of *Sq* and *Sdq* areal roughness parameters in a dedicated software developed in Matlab®. Initially, the dedicated software was validated against a commercial software. Afterwards, the calculation of *Sq* and *Sdq* parameters, as they are defined in the ISO 25178-2, was compared with the evaluation of the same parameters by the PSD. The results showed a broad agreement. It was found that differences were mostly due to the presence of noise. The evaluation of *Sq* and *Sdq* by the PSD is, in fact, less sensitive to noise. This was found above all for the *Sdq* parameter, where the approximation of the gradient in the conventional numerical evaluation can possibly enhance the influence of the noise. The PSD evaluation of *Sq* and *Sdq* was also proven more robust against different magnifications (namely different fields of view and pixel widths), retaining for the most unbiased statistical information for both 50× and 100× lens objectives. Thus, the PSD, and in general the frequency content of optical measurements, can be useful for the prediction of surface topographies based on digital modelling of measured data. It can be a manageable format of the acquired surfaces, less sensitive to noise and defects, to assist the digitalization of manufacturing.

Surface texture, Roughness Parameters, Power Spectral Density, Power Spectrum, *Sq*, *Sdq*

1. Introduction

Metrology for manufacturing is experiencing a shortage of adequate solutions to tackle the present revolutionary scenario in the manufacturing industry [1]. The fabrication of complex and advanced products requires novel metrology methods especially to assess the freeform structuring of manufactured components' surfaces and volumes [2–4].

Science and technology advances have made available new digital tools that are widely used in several fields of engineering. The digital twin is the concepts that mostly gained popularity [5]. The creation of a digital twin model from measured data can be an actual approach for dealing with the quality of complex products in manufacturing metrology. Nonetheless, such innovative modelling requires to be explored and harmonized with the existing techniques. The presented work investigated the topography modelling in the frequency domain, focusing on the extraction of *Sq* and *Sdq* roughness parameters, while dealing with the presence of noise. Noise and disturbances in general are nearly ubiquitous, affecting optical measurements above all at smaller scales. Thus, in the view of a fully digital system—i.e. without human intervention—the disturbance recognition is of central importance for an automated management of the measurements.

2. Methodology

The investigation initially compared the evaluation of the topographic noise among three different procedures, namely the measurement noise, the surface topography repeatability (STR), and the Allan deviation—mostly known as Allan variance. The measurement noise of optical instruments is defined in the ISO 25178-600 [6], while indications for its calculation are elsewhere [7].The STR is the equivalent of the standard deviation applied to a whole surface map of height values (pixel values) acquired by an optical instrument [8]. The STR is also equal to the measurement noise when evaluated on very smooth surfaces, while its value changes (normally increases) with different topographies.The Allan variance is a cluster analysis method, and recommended for correlated and auto-correlated measurements [9].

The different algorithms were applied to sequences of repeated acquisitions pixelwise, i.e. considering corresponding pixel values in the micrographs acquired by optical instruments. Thus, the results were extracted and compared to choose the most suitable indicator of the presence of noise in the measured topographies. The measurement noise was also considered combined with the residual flatness [6, 7]. In fact, they exist together as an amount to be overcome for having an actual detection of a surface topography.

Subsequently, the evaluation of *Sq* and *Sdq* parameters by power spectra was compared with the commercial software MountainsLab® (M-Lab) [10], and with an independent MATLAB® [11] implementation in agreement with the definitions in ISO 25178-2 [12].

Eventually, the frequency-domain calculation of *Sq* and *Sdq* was applied to two acquired sequences affected by disturbances, where respectively one and two micrographs produced outliers when averaging the pixel values.

2.1. Allan variance definition

A sequence of micrographs, as it is imaged by an optical instrument, is a non-stationary sequence, where the topography considered is a limited bandwidth of primary texture superimposed to the form of a limited area [13]. In addition, micrographs and pixel values are correlated. Therefore, the noise content of a sequence of micrographs is suitable to be detected by the Allan variance and deviation [14].

A sequence of N acquisitions was split in $M = \lfloor N/m \rfloor$ clusters, with $m = (1,2,\cdots,\lfloor N/2 \rfloor)$ [15]. Considering an average in each cluster $\overline{w}_k(m) = \frac{1}{m}\sum_{i=1}^{m} w_{(k-1)\times m+i}$ $(k = m)$, the Allan variance was evaluated as the sequence

$$\sigma_m^2 = \frac{1}{2(M-1)}\sum_{k=1}^{M-1}\left[\overline{w}_{(k+1)}(m) - \overline{w}_k(m)\right]^2 \quad (1)$$

The Allan deviation was analyzed as batch implementation, i.e. summing pixelwise the Allan variance contributors in the cluster sequence and afterwards computing the square root. Having the Allan deviation the same dimensions of a micrograph, it was also averaged among the pixels to obtain a value u_a that could be compared with the other quantities.

2.2. Spectral evaluation of Sq and Sdq

The 2D spatial Power Spectral Density (or power spectrum—PSD) was evaluated from the Fast Fourier Transform (FFT) h_{q_x,q_y} of a micrograph with dimensions ($L_x \times L_y$) as

$$C_{q_x,q_y}^{2D} = A^{-1}\left|h_{q_x,q_y}\right|^2 \quad (2)$$

where A is the micrograph definition area, $q_x = {}^{2\pi}/_{L_x}$ and $q_y = {}^{2\pi}/_{L_y}$ are the wavevectors, and the FFT was calculated using the Welch window. Thus, the roughness parameters were estimated as [16, 17]:

$$S_{q-PSD}^2 = A^{-1}\sum C_{q_x,q_y}^{2D} \quad (3)$$

$$S_{dq-PSD}^2 = A^{-1}\sum\left(q_x^2 + q_y^2\right)C_{q_x,q_y}^{2D} \quad (4)$$

3. Results

The main results are reported in the following tables. In some cases, the values in the tables are shown with more significant figures than what would have been required. This was done to allow an exhaustive numerical comparison of the different methods considered. The instruments used and their specifications are as follows:

- Zygo Nexview: coherent scanning interferometry (CSI); lens objectives—l.o.—20× (pixel size—p.s.—0.41 µm × 0.41 µm) and 50× (p.s. 0.16 µm × 0.16 µm—1024 × 1024 pixels for both lens objectives).
- Mahr MahrSurf: chromatic confocal (CC); l.o. 20× (p.s. 0.67 µm × 0.67 µm) and 50× (p.s. 0.27 µm × 0.27 µm—1198 × 1198 pixels for both lens objectives).
- Olympus Lext 4100: laser scanning confocal (LSC); l.o. 20× (p.s. 0.16 µm × 0.16 µm), 50× (p.s. 0.06 µm × 0.06 µm) and 100× (p.s. 0.03 µm × 0.03 µm—4096 × 4096 pixels for all lens objectives).

All the measurements were re-used micrographs from past projects, available in sets of twenty repeated measurements (unless indicated otherwise). They were all processed subtracting their least square plane, without applying any filtering. In this preliminary investigation and according to availability, the use of heterogeneous micrographs was intentional and as follows: 1) Different instruments measuring smooth surfaces for the noise qualification. 2) One instrument measuring different surfaces for *Sq* and *Sdq* qualification.

3.1. Noise qualification

The noise estimates are reported in the Tables 1–2. The measurement noise was evaluated by the "averaging method" [7] on a set of twenty repeated micrographs acquired at the same position of an optical-grade smooth surface (flat reference surface). The STR was evaluated on the same set. The residual flatness was instead evaluated on a set of twenty repeated micrographs acquired at different positions of the same flat reference surface [7]. Eventually, the averaged Allan deviation was evaluated on both sets of micrographs.

3.2. Sq and Sdq qualification

The surfaces adopted for the parameters qualification were: 1) Rubert standard 502 with irregular profile—type PRO in ISO 25178-70 [18]—and nominal *Ra* = 30 nm. 2) Rubert standard 529 with periodic sinusoidal shape (period 10 µm)—type PPS in ISO 25178-70 [18]—and nominal *Ra* = 100 nm. The micrographs were acquired by CSI (both 20× and 50× lens objectives). In addition to the standard deviation, both the median and the average were calculated. Disagreement between average and median, in fact, indicates the presents of possible outliers. Hence, the parameters calculation was performed by the commercial software, and in MATLAB according to the definitions in ISO 25178-2 and by (2)–(4). The results are in the Tables 3–10.

Table 1. Measurement noise, STR, residual flatness and averaged Allan deviation for CSI and CC using a 20× lens objective.

20× lens objective			CSI	CC
Noise (averaging)		u_N /nm	0.3	1.3
STR		u_{STR} /nm	0.2	1.3
Residual flatness		u_F /nm	0.4	4.1
Noise + res. Flat.		u_{NF} /nm	0.5	4.3
Allan dev.	Noise set	u_a /nm	0.4	2.4
	Flat. Set	u_a /nm	0.5	4.0

Table 2. Measurement noise, STR, residual flatness and averaged Allan deviation for LSC and CC using a 50× lens objective.

50× lens objective			LSC	CC
Noise (averaging)		u_N /nm	2.3	0.9
STR		u_{STR} /nm	2.2	0.9
Residual flatness		u_F /nm	7.3	2.9
Noise + res. Flat.		u_{NF} /nm	7.7	3.0
Allan dev.	Noise set	u_a /nm	3.3	2.4
	Flat. Set	u_a /nm	7.5	3.7

Table 3. *Sq* calculation on Rubert 502: Median, average, standard deviation (20× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 502—*Sq*, 20×	M-Lab	MATLAB	PSD
Median Sq_M /nm	39.37	39.37	38.18
Average Sq_m /nm	39.36	39.36	38.17
St. Dev. s_{Sqm} /nm	0.04	0.04	0.05
STR u_{STR} /nm	1.2		
Allan dev. u_a /nm	0.7		

Table 4. *Sq* calculation on Rubert 529: Median, average, standard deviation (20× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 529—*Sq*, 20×	M-Lab	MATLAB	PSD
Median Sq_M /nm	128.45	128.41	121.77
Average Sq_m /nm	128.52	128.51	121.74
St. Dev. s_{Sqm} /nm	0.78	0.78	0.30
STR u_{STR} /nm	22.9		
Allan dev. u_a /nm	11.5		

Table 5. *Sdq* calculation on Rubert 502: Median, average, standard deviation (20× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 502—*Sdq*, 20×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.0387	0.0388	0.0340
Average Sdq_m /1	0.0386	0.0390	0.0340
St. Dev. s_{Sdqm} /1	0.0001	0.0003	<0.0001
STR u_{STR} /nm	1.2		
Allan dev. u_a /nm	0.7		

Table 6. *Sdq* calculation on Rubert 529: Median, average, standard deviation (20× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 529—*Sdq*, 20×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.1785	0.1920	0.1428
Average Sdq_m /1	0.1791	0.1919	0.1436
St. Dev. s_{Sdqm} /1	0.0031	0.0020	0.0023
STR u_{STR} /nm	22.9		
Allan dev. u_a /nm	11.5		

Table 7. *Sq* calculation on Rubert 502: Median, average, standard deviation (50× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 502—*Sq*, 50×	M-Lab	MATLAB	PSD
Median Sq_M /nm	41.92	41.92	40.67
Average Sq_m /nm	41.92	41.92	40.67
St. Dev. s_{Sqm} /nm	0.05	0.05	0.05
STR u_{STR} /nm	0.8		
Allan dev. u_a /nm	1.2		

Table 8. *Sq* calculation on Rubert 529: Median, average, standard deviation (50× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 529—*Sq*, 50×	M-Lab	MATLAB	PSD
Median Sq_M /nm	118.50	118.52	118.39
Average Sq_m /nm	118.53	118.52	118.39
St. Dev. s_{Sqm} /nm	0.05	0.05	0.05
STR u_{STR} /nm	1.4		
Allan dev. u_a /nm	0.8		

Table 9. *Sdq* calculation on Rubert 502: Median, average, standard deviation (50× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 502—*Sdq*, 50×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.0538	0.0542	0.0507
Average Sdq_m /1	0.0538	0.0542	0.0507
St. Dev. s_{Sdqm} /1	0.0001	0.0001	0.0001
STR u_{STR} /nm	0.8		
Allan dev. u_a /nm	1.2		

Table 10. *Sdq* calculation on Rubert 529: Median, average, standard deviation (50× lens objective). The reported STR and averaged Allan deviation are related to the whole set of micrographs.

Rubert 529—*Sdq*, 50×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.0986	0.0984	0.0909
Average Sdq_m /1	0.0987	0.0984	0.0909
St. Dev. s_{Sdqm} /1	0.0006	0.0003	0.0006
STR u_{STR} /nm	1.4		
Allan dev. u_a /nm	0.8		

3.3. Surface analysis

The measurements analyzed were acquired on a steel component (A1), polished by diamond buff (grade 15) and surface finish with nominal *Ra* in the interval 50–76 nm. The micrographs were measured by LSC. They were five repeated acquisitions by 50× lens objectives and fifteen by 100×, both in the same position on A1.

The high values of the Allan deviations highlight the presence of noise. In the case of 50× measurements, in fact, the disturbances led to one outlier micrograph, with abnormal *Sq* and *Sdq* values. Two were instead the outlier micrographs for the 100× measurements. The outlier micrographs are in the Figures 1–2, represented in the frequency domain and compared with the average of the respective sets of measurements. To simplify the visual inspection, the 2D PSD is pictured in the figures as split in two one-sided 1D PSD. In addition, the pixelwise average of the 100× set of measurements is shown in Figure 3, while in Figure 4 there is the corresponding Allan deviation. It indicates the average distribution of the noise in the overall sequence of acquired micrographs. Eventually, the results are summarized in the Tables 11–14 for the three software implementations.

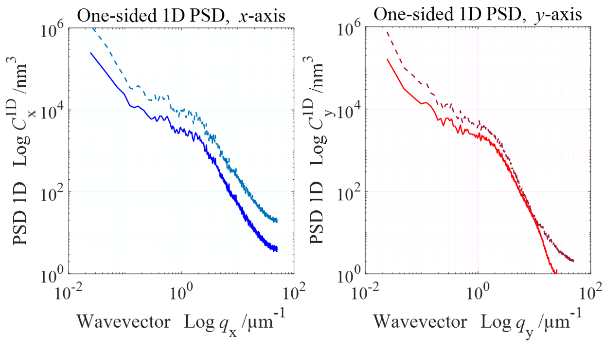

Figure 1. Average PSD of the steel component 50× set of measurements, split along the *x*- and *y*-axes (solid lines) and compared with the PSD of the outlier micrograph (dashed lines).

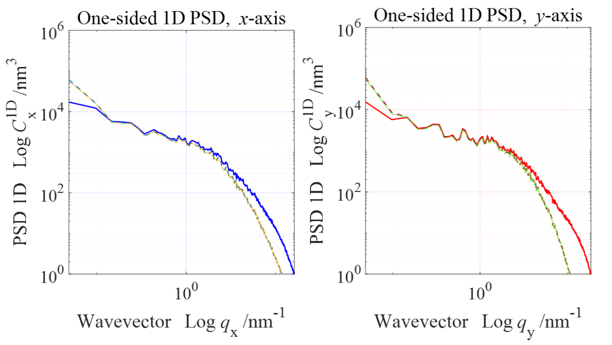

Figure 2. Average PSD of the steel component 100× set of measurements, split along the *x*- and *y*-axes (solid lines) and compared with the PSD of the outlier micrographs (dashed and dotted lines).

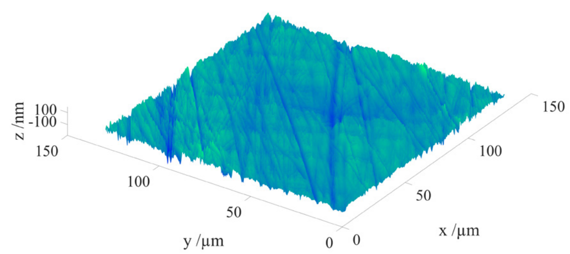

Figure 3. Pixelwise average of the steel component 100× set of measurements.

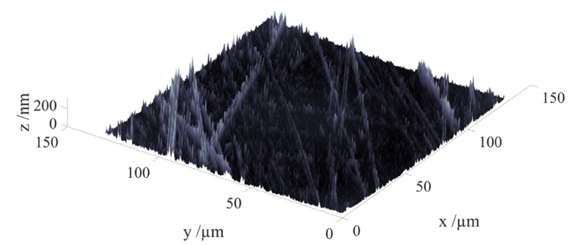

Figure 4. Batch implementation of the Allan deviation of the steel component 100× set of measurements.

Table 11. *Sq* calculation on A1: Median, average, standard deviation (50× lens objective) evaluated on 5 repeated measurements. The averaged Allan deviation quantifies the noise, including one outlier micrograph (M-Lab average without outlier $Sq = (49 \pm s_m)$ nm, $s_m < 1$ nm; PSD average without oulier $Sq = (45 \pm s_m)$ nm, $s_m < 1$ nm).

A1—*Sq*, 50×	M-Lab	MATLAB	PSD
Median Sq_M /nm	50	50	45
Average Sq_m /nm	96	96	59
St. Dev. s_{Sqm} /nm	105	105	32
Allan dev. u_a /nm	93		

Table 12. *Sdq* calculation on A1: Median, average, standard deviation (50× lens objective) evaluated on 5 repeated measurements. The averaged Allan deviation quantifies the noise, including one outlier micrograph (M-Lab average without outlier *Sdq* = 0.152 ± 0.001; PSD average without outlier *Sdq* = 0.090 ± 0.001).

A1—*Sdq*, 50×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.152	0.154	0.090
Average Sdq_m /1	0.344	0.327	0.118
St. Dev. s_{Sdqm} /1	0.428	0.388	0.064
Allan dev. u_a /nm	93		

Table 13. *Sq* calculation on A1: Median, average, standard deviation (100× lens objective) evaluated on 15 repeated measurements. The averaged Allan deviation quantifies the noise, including two outliers micrographs (M-Lab average without outliers *Sq* = (50 ± 1) nm; PSD average without outliers *Sq* = (45 ± s_m) nm, s_m < 1 nm).

A1—*Sq*, 100×	M-Lab	MATLAB	PSD
Median Sq_M /nm	50	50	45
Average Sq_m /nm	51	51	47
St. Dev. s_{Sqm} /nm	3	3	6
Allan dev. u_a /nm	40		

Table 14. *Sdq* calculation on A1: Median, average, standard deviation (100× lens objective) evaluated on 15 repeated measurements. The averaged Allan deviation quantifies the noise, including two outliers micrographs (M-Lab average without outliers *Sdq* = 0.185 ± 0.004; PSD average without outliers *Sdq* = 0.103 ± 0.002).

A1—*Sdq*, 100×	M-Lab	MATLAB	PSD
Median Sdq_M /1	0.185	0.185	0.103
Average Sdq_m /1	0.176	0.177	0.098
St. Dev. s_{Sdqm} /1	0.024	0.024	0.014
Allan dev. u_a /nm	40		

4. Discussion

It can be seen from the Tables 1–2 that averaging method and STR are equivalent for the evaluation of the measurement noise. Moreover, the combined contributors of noise and residual flatness are equivalent to the averaged Allan deviation when this is evaluated on the residual flatness set of measurements. From Tables 3–10 it can also be seen that STR and averaged Allan deviation have similar trend when evaluated on measurements from surfaces other than flat references. In details, the STR evaluates the variability of an acquired sequence, and both its matrix implementation and the averaged version are suitable contributors in an uncertainty budget. Even so, STR cannot locate the presence of the disturbances on a micrograph. On the contrary the Allan deviation is sensitive locally to disturbances, while it tends to small values if no significant effects are detected in the micrographs. Therefore, the Allan deviation was chosen as indicator of the amount of disturbances in the last part of the investigation.

The calculation of *Sq* and *Sdq* parameters is in large agreement among the three different evaluations (see Tables 3–10). Differences can be noticed for *Sdq* parameter, which tends to be lower for the PSD values. This is enhanced by the presence of noise (see Table 6). In such case, differences of *Sdq* arise also between M-Lab and Matlab values, possibly due to different approximations of the gradient in the numerical evaluation, and also to different influence of the noise in the least square calculation of the levelling plane. To conclude, the PSD evaluation is more robust in the presence of strong disturbances (see Tables 11–14). This is especially true for Sdq, which also has much lower standard deviation than the regular evaluation.

5. Conclusions

This preliminary investigation has evidenced a robust agreement between the surface assessment according to the areal method and the one in the frequency domain. Most importantly, the evaluation in the frequency domain maintains the measurements statistical content and appears more robust because connected with the form of the spectrum and not much with the pixels distribution and/or their number. Moreover, the micrographs assessment in the presence of noise often requires visual inspections, heavy filtering and manual processing. The Allan variance can be useful to locally detect and eliminate disturbances. Thus, this certainly opens to the possibility of a fully automated management of surfaces acquisition and processing. Nevertheless, more work is needed for a systematic generalization of the presented results and of their applicability. The analysis of factors like the influence of the FFT window on the PSD parameters calculation and the integration of an uncertainty budget are important insights for future work.

References

[1] Przyklenk A, Balsamo A, O'Connor D, Evans A, Yandayan T, Akgöz SA, Flys O, Phillips D, Zeleny V, Czułek D, Meli F, Ragusa CS and Bosse H 2021 New European Metrology Network for advanced manufacturing *Meas. Sci. Technol.* **32** 111001

[2] Brown CA, Hansen HN, Jiang XJ, Blateyron F, Berglund J, Senin N, Bartkowiak T, Dixon B, Le Goïc G, Quinsat Y, Stemp WJ, Thompson MK, Ungar PS and Zahouani EH 2018 Multiscale analyses and characterizations of surface topographies *CIRP Annals* **67-2** 839–862

[3] Brinksmeier E, Karpuschewski B, Yan J and Schöneman L 2020 Manufacturing of multiscale structured surfaces *CIRP Annals* **69-2** 717–739

[4] Jiang X, Senin N, Scott P J and Blateyron F 2021 Feature-based characterisation of surface topography and its application *CIRP Annals* **70-2** 681–702

[5] Jones D, Snider C, Nassehi A, Yon J and Hicks B 2020 Characterising the Digital Twin: A systematic literature review *CIRP Journal of Manufacturing Science and Technology A* **29** 1755–5817

[6] ISO 25178-600:2019 Geometrical product specifications (GPS) – Surface texture: Areal—Part 600: Metrological characteristics for areal topography measuring methods. ISO 25178-600 (Geneva: International Organization for Standardization)

[7] Giusca C L, Leach R K, Helary F, Gutauskas T and Nimishakavi L 2012 Calibration of the scales of areal surface topography-measuring instruments: part 1. Measurement noise and residual flatness *Meas. Sci. Technol.* **23** 035008

[8] ISO 25178-604:2013 Geometrical product specifications (GPS) – Surface texture: Areal—Part 604: Nominal characteristics of non-contact (coherent scanning interferometry) instruments. ISO 25178-604 (Geneva: International Organization for Standardization)

[9] JCGM 100:2008 Evaluation of measurement data – Guide to the expression of uncertainty in measurement Joint Committee for Guides in Metrology, Bureau International des Poids et Mesures (BIPM), Sevres, France

[10] www.digitalsurf.com

[11] www.mathworks.com

[12] ISO 25178-2:2021 Geometrical product specifications (GPS) – Surface texture: Areal—Part 2: Terms, definitions and surface texture parameters. ISO 25178-2 (Geneva: International Organization for Standardization)

[13] Sayles R and Thomas T 1978 Surface topography as a nonstationary random process *Nature* **271** 431–434

[14] Zhang F N 2008 Allan variance of time series models for measurement data *Metrologia* **45** 549

[15] Lv P, Liu J, Lai J and Huang K 2015 Allan variance method for gyro noise analysis using weighted least square algorithm *Optik* **126-20** 2529–2534

[16] Persson B N J, Albohr O, Tartaglino U, Volokitin A I and Tosatti E 2005 On the nature of surface roughness with application to contact mechanics, sealing, rubber friction and adhesion *J. Phys.: Condens. Matter* **17** R1

[17] Jacobs T D B, Junge T and Pastewka L 2017 Quantitative characterization of surface topography using spectral analysis *Surf. Topogr.: Metrol. Prop.* **5** 013001

[18] ISO 25178-70:2014 Geometrical product specification (GPS) – Surface texture: Areal—Part 70: Material measures. ISO 25178-70 (Geneva: International Organization for Standardization)