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Experimental approach to establishing a model of nanoscale friction

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Abstract
The main limitation in modelling nanoscale friction is the variety of physicochemical processes and their interactions in nanoscale contacts that depend on the materials and on the conditions relating to sliding velocity, normal forces, temperature etc. To assess the value of the nanoscale friction coefficients, in this work an experimental methodology using a scanning probe microscope (SPM) in the lateral force microscopy (LFM) mode is hence used on various thin film samples. The measurements are designed by employing the centroidal Voronoi tessellation technique with 50 sample points. By using Support Vector Machine-based machine learning, the trends of the values of the friction coefficients can thus be established despite the marked stochastic contributions, creating therefore the preconditions for obtaining a multi-dimensional model relating the value of nanometric friction to its influencing parameters.

Nanoscale friction, experimental determination, scanning probe microscope, nonlinear model, machine learning

1. Introduction

Friction with its stochastic nonlinear characteristics often limits the performances of micro- and nanodevices. The available friction models do not take into account all the physical phenomena involved in nanoscale contacts that comprise physicochemical processes and their interactions that, in turn, depend on a variety of process parameters comprising: the materials in contact, sliding velocity, normal forces, temperature etc. [1]. In this work, the experimental determination of the dependence of nanometric friction on these parameters is carried out via SPM in LFM mode. Due to the large number of monitored influences, the number and type of measurements is determined by using metamodeling techniques. Analyses of the obtained data, performed via advanced mathematical tools, allow hence obtaining the trends of the values of the friction coefficients (CoFs), creating thus the preconditions for obtaining a multi-dimensional model of nanoscale friction.

2. Experimental methodology

The experimental assessment of friction on the nanometric scale is performed in this work by using the Bruker Dimension Icon SPM. To tune the measurement conditions and quantify the obtained results, a precise calibration of probes' bending and torsional stiffness is needed. The probe's geometry is hence determined via accurate measurements from SEM micrographs, and corresponding analytical and FEM calculations, are performed. The obtained results allow establishing that the uncertainty of the stiffness values is significant (up to ± 15 %) [2]. To constrain the influence of tip wear on adhesion, and thus on the value of nanoscale friction, during the performed measurements the sliding distance with a single tip is then also limited.

The hence analysed samples are: fused silica (FS), highly oriented pyrolytic graphite (HOPG), Al_2O_3, TiO_2, MoS_2, stainless steel (SS of type X39CrMo17-1) and Al. Al_2O_3 and TiO_2 films are synthesised via atomic layer deposition (ALD) on a Beneq TFS 200 device. The used precursor species are, respectively, trimethylaluminium ($Al(CH_3)_3$) and titanium-tetrachloride ($TiCl_4$) in combination with H_2O, while high-purity N_2 is used as the purging gas. The deposition of Al_2O_3 is carried out at 200 °C with the following ALD cycle: 180 ms $Al(CH_3)_3$ pulse, 1 s purge, 180 ms H_2O pulse, 1 s purge. For the TiO_2 deposition at 150 °C the pulsing times for $TiCl_4$ and H_2O are, respectively, 250 ms and 180 ms, followed by purging cycles of, respectively, 3 s and 2 s. The Al, SS and MoS_2 thin films are, in turn, obtained by using pulsed laser deposition (PLD). The employed Nd:YAG laser parameters are: wavelength 1064 nm, pulse duration 4 ns @ 5 Hz, pulse energy 340 mJ. Laser pulses are focused on the target that is parallel to the Si substrate and inclined by 45° with respect to the impinging laser beam, yielding a fluence of 18 J/cm^2. 5 000 laser pulses are hence used to obtain the adopted 150 µm film thickness. The distance between the target, which is rotated to avoid drilling and increase films' homogeneity, and the substrate is 3 cm. The target holder and the substrate are kept on a floating potential at room temperature in a high vacuum environment. To determine finally the atomic concentration of the obtained films and the eventual residual condensed water vapour layer thickness on films' surfaces, prior to the actual measurements the samples are characterized via X-ray photoelectron spectroscopy.

3. Design of experiments

The considered parameters influencing nanoscale friction on the described samples and their value ranges are: normal force F_N = 10 nN… 150 nN, sliding velocity v = 5 nm/s … 500 nm/s and temperature ϑ = 20 °C … 80 °C. Design of experiment (DoE) is thus conducted by defining the experimental space via sampling methods that enable the development of a meta-model. Since recent studies indicate that among these centroidal Voronoi tessellation (CVT) [3] has several advantages, CVT is used to generate 50 sample points. Given the set of desired points ("generators") and a distance function from each generator to its mass centroid, Voronoi tessellations are subdivisions of the 3D experimental space. The variation of the influencing parameters is hence defined via a discrete uniform distribution, i.e., a distribution where a finite number *n* of homogeneously spaced values has the same probability to be observed [3-4]. The integer parameters of the distribution are:

$$n = b - a + 1 \qquad (1)$$

where *a* and *b* are the lower and upper limit of the values of the considered parameter. The distribution of sample points is thus generated by a discrete probability distribution *k* attained by using a probability mass function *f*(*k*) defined in equation (2), while the cumulative distribution function *F*(*k*) given by equation (3) is used to specify the placement of multivariate random variables (i.e. the points in the considered multi-dimensional influencing parameters' space) [3-4]:

$$f(k) = \begin{cases} 1/n & \text{if } a \le k \le b \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

$$F(k) = \begin{cases} 0 & \text{if } k < a \\ \dfrac{\lfloor k \rfloor - a + 1}{n} & \text{if } a \le k < b \\ 1 & \text{if } k > b \end{cases} \qquad (3)$$

Given a density function, the centre of mass of each subset making up the Voronoi tessellation can thus be determined. Since, however, generally the locations of the generators do not coincide with the centres of mass of the data subsets, distinct Voronoi tessellations called CVTs are used to assure the convergence of these locations [3-4]. To gain insight into the stochasticity of the measured friction coefficients, 5 repetitive measurements are performed in each measurement point.

4. Data analysis

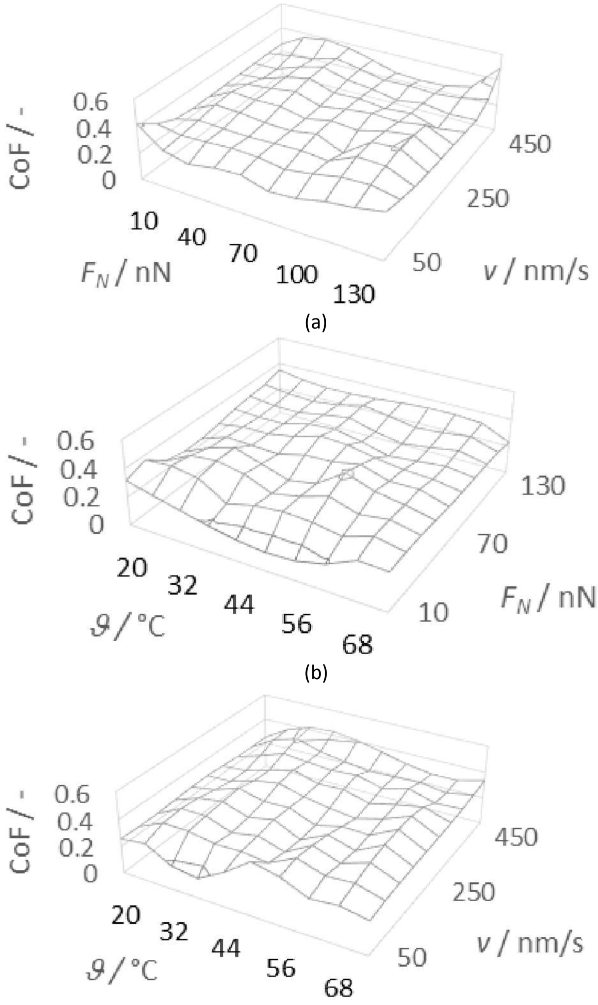
The data resulting from the described measurements, characterised by discrepancies in repetitive measurements of up to ± 12 %, is analysed using the commercially available GoSumD software. The software is based on recently developed machine learning computational algorithms for nonlinear model representation that enable a simultaneous examination of global uncertainties and contributions of a large number of parameters. In fact, these predictive algorithms map the input values into higher-order hyperplanes, where optimisation routines are used to achieve an easier and efficient localised regression minimisation [4]. The thus achieved analytical representation of the function describing the nanoscale CoFs in the considered multi-dimensional hyperspace, defined by correlation coefficients corresponding to the 50 measured points, can be used to predict the CoF values in the whole considered range of the influencing parameters.

In Fig. 1. are thus, as an example of the obtained results, mapped the predicted values of the nanoscale CoFs attained on TiO_2 samples. The depicted 3D surfaces are generated by interpolating (fitting) the data points in the CVT four-dimensional hyperplanes via the Renka-Cline interpolation [5]. Since several patterns start appearing from the measurements, these plots show some typical features of the attained data:

- when ϑ is kept constant, for the lowest and the highest considered *v* and F_N values, CoF values tend to increase;
- when *v* is kept constant, the CoFs tend to markedly decrease for the lowest F_N values, with a CoF valley for $\vartheta \approx 40$ °C;
- when F_N is kept constant, for $\vartheta \approx 30$ °C there is a CoF valley for the smallest *v* values and a CoF peak for the highest considered *v* values.

5. Conclusions and outlook

The progress on a structured experimental approach aimed at determining the dependence of nanoscale friction on a range of influencing parameters is outlined in this work. The developed experimental methodology, coupled with DoE methods and an elaborated mathematical processing of attained data, allows obtaining a good prediction of nanometric frictional behaviour in a multi-dimensional space, despite the marked stochastic variability of the measurements. What is more, interesting typical features start appearing in the determined CoF values over the whole range of considered materials. This creates thus the preconditions for obtaining a comprehensive model relating the value of nanoscale friction to its influencing parameters and their relative impact. All of this constitutes the basis for the possibility to extend the applicability of established friction models to the nanometric range, thus advancing further micro and nano electro-mechanical systems and precision engineering.



(c)

Figure 1. CoF values on a TiO_2 sample with fixed: $\vartheta = 20$ °C (a), $v = 250$ nm/s (b) and $F_N = 50$ nN (c).

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