Marko Perčić,[1, 2, 3] *Saša Zelenika*[1, 2, 3] *and Igor Mezić*[2, 4]

Characterization of influential parameters on friction in the nanometric domain using experimental and machine learning methods

[1] University of Rijeka, Faculty of Engineering, Vukovarska 58, 51000 Rijeka, CROATIA
[2] University of Rijeka, Centre for Micro- and Nanosciences and Technologies, Radmile Matejčić 2, 51000 Rijeka, CROATIA
[3] University of Rijeka, Center for Artificial Intelligence and Cybersecurity, Radmile Matejčić 2, 51000 Rijeka, CROATIA
[4] UC Santa Barbara, Department of Mechanical Engineering, Santa Barbara, CA 93105, USA

Abstract

Friction is a ubiquitous phenomenon of great research interest in engineering practice. Fundamental frictional features of two solids in contact and in relative motion are governed by microscopic single asperity contacts at their interface. A structured multidisciplinary approach to the experimental determination of friction in the nanometric domain is presented in this work. The dependence of nanoscale friction on process parameters comprising the materials in relative motion, normal forces, sliding velocities and the temperature conditions is studied experimentally by employing scanning probe microscopy. The data hence attained from multidimensional experimental measurements on thin-film samples is used for the development of machine learning-based models. In fact, due to the stochastic nature of the considered phenomena, conventional regression methods yield poor predictive performances, prompting thus the usage of the machine learning numerical paradigm. Such an approach enables obtaining an insight into the concurrent influence of the process parameters on nanoscale friction. A comparative study allows thus showing that, while the best typical regression models result in coefficients of determination (R^2) of the order of 0.3, the predictive performances of the used machine learning models, depending on the considered sample, yield R^2 in the range from 0.54 to 0.9. The proposed method, aimed at accomplishing an in-depth insight into the physical phenomena influencing nanoscale frictional interactions, will be complemented next with advanced studies based on genetic programming-based artificial intelligence methods. These could, in fact, allow obtaining a functional description of the dependence of nanoscale friction on the studied variable parameters, thus enabling not only true nanoscale friction prediction but also an important tool for control purposes.

Keywords: *nanoscale friction, experimental methodology, scanning probe microscopy, thin films, data mining, machine learning, artificial intelligence*

1. Introduction

Devices characterised by micro- and nanopositioning precision are often required in precision engineering as well as in micro- and nanosystems' technologies. When conventional devices based on sliding and rolling mechanisms are used in this frame, positioning precision is mostly limited by friction with its stochastic nonlinear characteristics [1]. Frictional phenomena on the macro- and meso-scales are described quite well in prior art, enabling their effects to be simulated via suitable models, as well as proficiently compensated via proper control typologies [2-3]. On the other hand, however, the available friction models do not take into due account true nanometric motions or the scaling phenomena related to friction [4]. In fact, the understanding of friction at the level of atomic interactions was enabled only in the last 20 to 30 years by the availability of scanning probe microscopy (SPM) methods [5], which enable experimental investigations of frictional single-asperity contacts [6].

A structured multidimensional experimental approach is thus developed in this work to study the dependence of the nanoscale friction force F_f on different concurrently varying process parameters comprising the materials in relative motion, normal forces F_N, sliding velocities v and temperatures ϑ.

Technologies (NANORI) of the University of Rijeka, Croatia [8]. The data obtained on thin-film samples is then used for the development of machine learning-based nanoscale friction models with the aim of gaining a deeper insight into the physical phenomena that influence nanotribological interactions.

2. Experimental set-up

The used experimental procedure involves SPM in the lateral force microscopy (LFM) mode (Figure 2), enabling measurements on Al_2O_3 and TiO_2 thin-film samples synthesized via atomic layer deposition (ALD) [9] at the NANORI premises, as well as Al, MoS_2

Fig. 1. Bruker Dimension Icon SPM

and stainless steel X39CrMo17-1 thin-film samples synthetized by using pulsed laser deposition (PLD) [10] at the Institute of physics in Zagreb, Croatia. Lateral (transversal) scans are hence performed on 500 x 500 nm^2 surfaces of the analysed samples, inducing a torsion of the cantilever bearing the measurement tips [11]. The resulting voltages are converted to values of the lateral (transversal) force exerted on the sample by calibrating the mechanical behaviour of the probe itself by using multiple methods, comprising the calibration based on using the TGF11 calibration sample [12], finite element modelling (FEM) and analytical calculations [6]. It was hence established that calibration is strongly dependant on the actual dimensions of the cantilevers. Considering that these dimensions are in micrometric range, while the production process of the probes inherently prevents the achievement of uniform dimensions in the whole production batch, calibration generally constitutes a hard and tedious task [6].

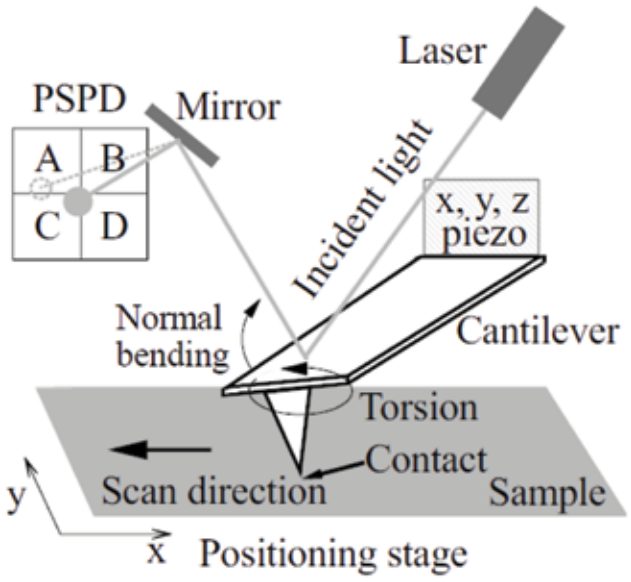


Fig. 2. Scheme of the LFM measurement configuration [6]

3. Definition of the measurement points

The considered parameters influencing nanoscale friction on the described samples, and their respective 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) [13] has several advantages, CVT is used to generate 50 sampling points in the considered multidimensional experimental space.

Given the set of desired points ("generators") and a distance function from each generator to its mass centroid, Voronoi tessellations are then subdivisions of the thus defined experimental space. The variation of the influencing parameters is herein 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 [13]. The integer parameters of the distribution are:

$$n = b - a + 1 \tag{1}$$

where a and b are the lower and upper limit of the values of the considered parameter.

A 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). The cumulative distribution function $F(k)$, given by equation (3), is, in turn, used to specify the placement of the multivariate random variables (i.e., the points in the considered multidimensional influencing parameters' space):

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

$$F(k) = \begin{cases} 0 & \text{if } k < a \\ \frac{[k]-a+1}{n} & \text{if } a \le k < b \\ 1 & \text{if } k > b \end{cases} \tag{3}$$

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 [13].

To gain insight into the stochasticity of the measured friction coefficients, five repetitive LFM measurements

are then performed in each of the 50 measurement points defined via the above DoE procedure [6].

4. Experimental results

Besides calibration, the inherent difficulties in the considered measurement procedure are amplified by synergetic effects occurring in the nanometric contact region, comprising the inevitable wear of the tip, thermal dilatations, and effects induced by the adhesive forces F_A. The latter proved to be especially tedious, since it has a strong nonlinear dependence on temperature on its own. It was hence determined that in the herein considered cases the correlation factor linking the LFM voltage readings to the corresponding nanoscale friction force values can vary by a whole order of magnitude. On the other hand, the wear of the used tips induces the necessity to use a fresh tip after every 50 LFM measurement cycles. The experimental methodology developed in this work in any case not only takes into account all these effects, but also limits their influence on measurements' uncertainties [6].

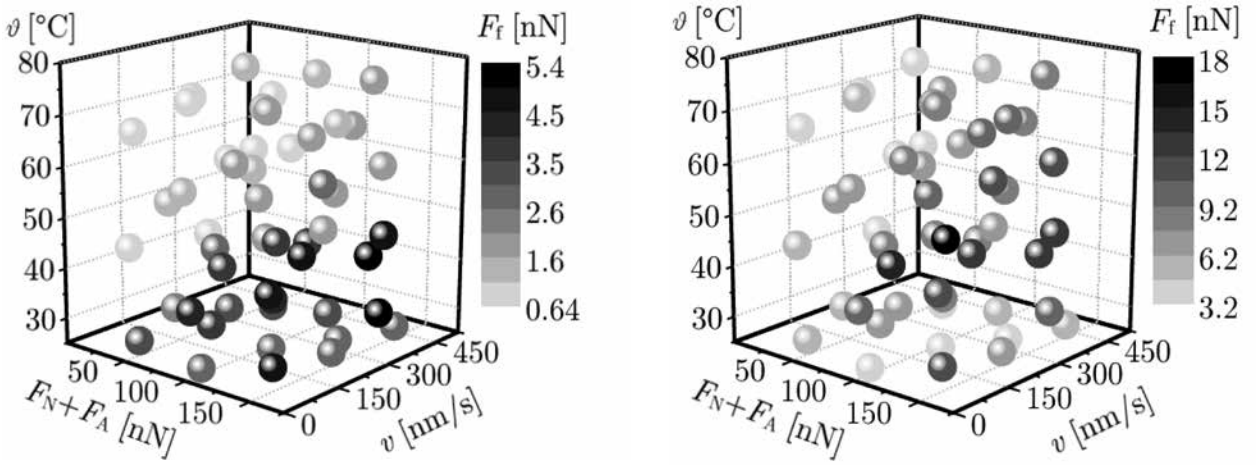
After taking into account the adhesion-corrected calibration factors, the obtained LFM scan signals are analysed in order to obtain the actual nanoscale friction force F_f in the 50 measurement points defined by employing the described CVT DoE methodology. The thus determined F_f values are shown, as typical result for the ALD and the PLD synthesized samples, in the colour-coded plots of Figure 3. In Figure 3a are thus depicted the results attained for the Al_2O_3, and in Figure 3b for the MoS_2 sample, respectively [6]. The results allowed also evidencing the noticeable stochastic nature of frictional phenomena, which makes the modelling based on this data, using conventional methods, difficult. The results allow establishing first-order rough correlations between the multiple studied influencing parameters and the resulting F_f values but, to determine systematic and reliable correlations, advanced mathematical tools have to be used [6].

5. Modelling nanoscale friction

Empirical insights obtained via the above thorough experimental procedure [6], are used as a basis for the development of a predictive model of nanoscale friction. The data collected in the 50 experimental measurement points, defined by employing the CVT DoE methodology, are hence used as the main dataset for the development of appropriate friction models. Each models' predictive performance is tested subsequently by employing the same experimental technique on a separate set of 15 measurement points defined randomly by using the Monte Carlo (MC) method [14].

Modelling is therefore primarily carried out using the conventional methods of regression analysis, i.e, linear, nonlinear, multivariate regression methods etc., but, due to the evidenced stochastic nature of the considered nanotribological phenomena, they yield poor results in describing the obtained experimental data, and even weaker predictive performances.

A machine learning (ML) paradigm is thus adopted to obtain an insight into the studied complex, multidimensional interactions and obtain a predictive model of nanoscale friction according to the schematics shown in Figure 4 [15]. Generally, ML algorithms for regression problems provide a so-called



(a) (b)

Fig. 3. Colour-coded distributions of experimental F_f values for the 50 CVT DoE points for the Al_2O_3 (a), and MoS_2 (b) samples with adhesion-corrected total load F_N+F_A [6]

black-box solution with predictive results. The models thus developed are based on the TensorFlow [16], Scikit-learn [17] and GoSUMD [18] implementations. The herein used ML algorithms are thus additive regression, stacking and bagging classifiers, lazy algorithms, multi-layer perceptron (MLP), support vector regression (SVR), decision trees and random forest (RF) ensembles [19]. These methods are used for obtaining important insights into the analysed experimental space trough visualization analyses, providing important knowledge for further studies but, unfortunately, do not result in a functional mathematical form of the underlying relationships.

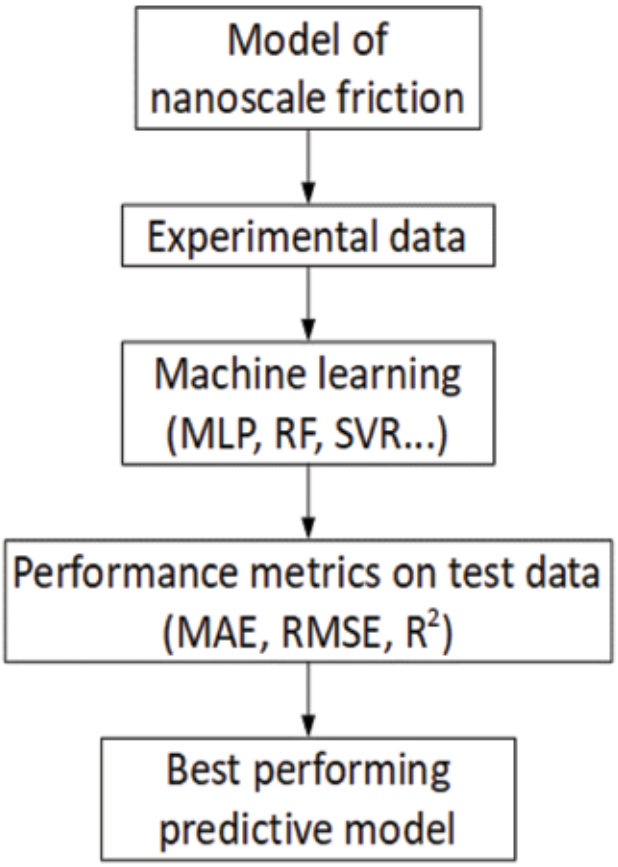


Fig. 4. Methodology for the development of ML-based predictive models of nanoscale friction

By employing binary encoding for the material class, the developed ML models are trained on the complete CVT-based dataset for each material separately, as well as on a combined (pooled) dataset pertaining to all studied materials, subjected in all cases to a 10-fold cross-validation. The ML models are then thoroughly assessed on the mentioned separately measured MC-based experimental dataset – the test dataset. To ensure realistic (habitual) conditions of the samples, these measurements are conducted, in contrast to the main CVT DoE-based measurements, without drying the samples prior to the measurements. Coupled to the

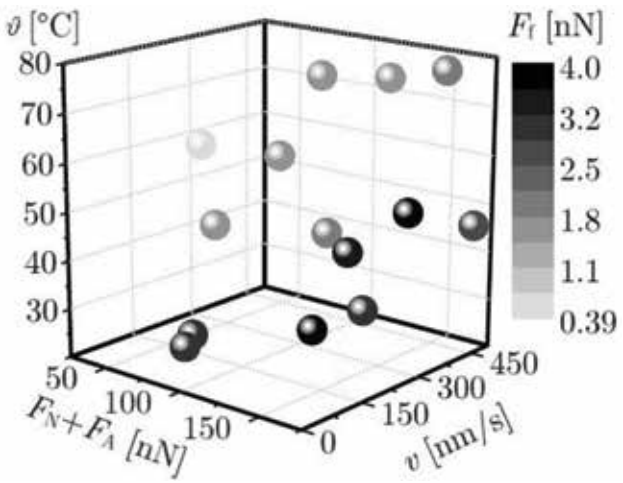


Fig. 5. Colour-coded distribution of experimental F_f values for the test dataset of 15 MC-based points for Al_2O_3 [15]

random distribution of the 15-point test dataset, the thus performed measurements, shown in Figure 5 for the Al_2O_3 thin-film sample, assure thus truthful F_f values that provide, moreover, the most difficult predictive task for developed models.

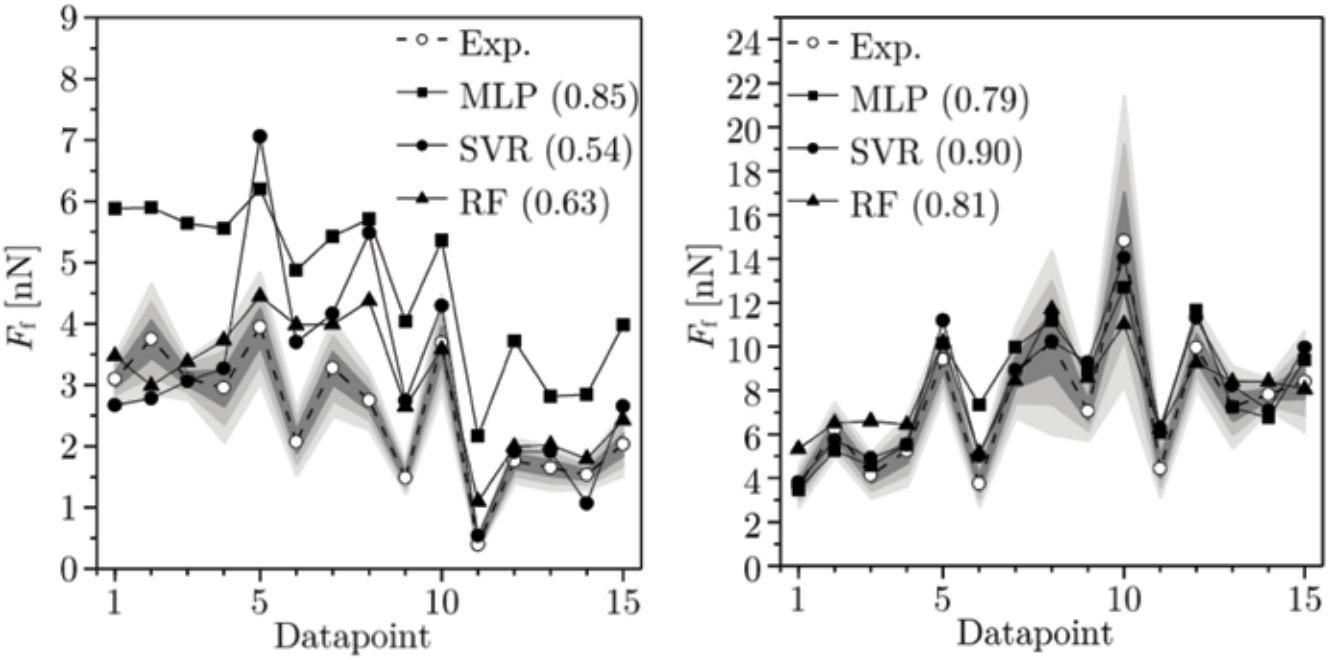
Each models' predictive performances are finally analysed by using performance metrics consisting of the mean absolute (MAE) as well as root mean square (RMSE) errors, and the respective coefficients of determination (R^2) [15].

6. Results and discussion

All developed ML models show far better predictive performance (higher R^2) than the conventional regression methods that yield R^2 in the range of ca. 0.3. What is more, all ML models, developed by training on a pooled (combined) dataset, comprising data acquired experimentally on multiple samples, show a higher level of predictive performances.

The finally obtained predictive performances on the MC-based test dataset are shown in Figure 6 for each of the best performing developed ML model. The respective R^2 values are reported in the Figure in parenthesis. In Figure 6 are depicted also the attained uncertainty levels in three shades of grey, representing, respectively, the variance of data ($\pm 1\sigma$ as the darkest, $\pm 2\sigma$ as the medium and $\pm 3\sigma$ as the lightest shade of grey that presents, with empirical near-certainty, all data).

For the Al_2O_3 thin-film sample synthesized via the ALD technique, in Figure 6a it can thus be evidenced that, even though the MLP algorithm results in high R^2



(a) (b)

Fig. 6. Predictive performances of the considered ML models on the MC test dataset for the Al_2O_3 (a), and MoS_2 (b) samples [15]

values, it is visually far quite far away from the experimental data. The RF and SVR predictions follow, in turn, the experimentally obtained data much better. In the case of the MoS_2 sample synthetized by using the PLD methodology, the test data predictions shown in Figure 6b allow noting much better predictive performances for all the ML models. The SVR algorithm captures in this case 90 % of the variance of F_f.

Such considerations allowed, therefore, concluding that the developed ML models allow providing effective predictions of the influence of the multiple concurrently acting process parameter on the value of the friction force with satisfactory levels of accuracy, i.e., with R^2 values ranging from a minimum 0.54 for the SVR algorithm on the Al_2O_3 sample, to a maximal value of 0.9 for the SVR prediction on the MoS_2 sample.

Although the developed ML models provide, thus, generally good predictive performance, their practical usage is quite limited by their inherent black-box nature. Further research has thus to be focused on obtaining models that allow obtaining mathematical expressions which will have equally good (or better) predictive performance as the ML models, but will enable practical usage in developing suitable control typologies that will allow an active compensation of nanotribological effects.

7. Conclusions and outlook

The activities and topics described in this work provide an overview of the obtained experimental and numerical results in the ongoing research effort on frictional phenomena in the nanometric domain carried on at the University of Rijeka, Croatia. The developed experimental methodology allows for the first time to determine the concurrent influence of multiple variable process parameters on the value of the nanoscale friction force.

The attained measurement results imply, however, the necessity of developing also suitable mathematical modelling tools, since the multidimensionality and the stochastic nature of the studied phenomena are an evident challenge for the conventional modelling methods. The analysis of the obtained measurements is thus performed by using state-of-the-art black-box ML models. It is hence established that their predictive performances can generally be considered satisfactory, but their practical applicability is limited, since they do not allow to obtain explicit functional dependencies of nanoscale friction on the multiple considered variable process parameters.

Further numerical analyses, based on employing novel genetic programming-based artificial intelligence (AI) methods are hence needed to fully characterize the influencing effects of nanoscale friction through a mathematical expression. Preliminary results obtained

in this frame are comforting since, despite the evidenced complexity of the herein studied phenomena, the AI-based symbolic regression models [20] could allow attaining excellent predictive performances, but indeed result also in a simple functional description of the multidimensional dependence of nanoscale friction on the studied variable influencing parameters. An operational and efficient tool for nanoscale friction prediction, for further scientific and technological analyses, but also for eventually enabling the compensation of frictional effects via appropriate adaptive control typologies, could thus be on the verge of being successfully obtained.

What is more, further studies on the considered topics are focused on bridging the multiscale gap in tribological studies, ranging from atomic and molecular to micro- and macroscales. To provide further and deeper insights into the fundamental principles of friction, the current efforts of our research group are therefore also directed towards active cooperation with the Molecular biology and nanotechnology laboratory (MoIBNL) at the University of Trieste, Italy, [21] on molecular dynamic studies of nanoscale friction phenomena.

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