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Multivariate AI-based predictive model of nanoscale friction

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Abstract
As a major source of uncertainties in micro- and nanopositioning devices, friction, characterised by complex stochastic phenomena, is one of the major challenges in developing reliable predictive models od systems' behaviour. Based on recently performed lateral force microscopy experimental measurements of thin films' nanoscale friction, fundamental frictional mechanisms in atomic-scale single-asperity contacts are investigated in this work vs. the concurrent influence of multivariate process parameters. The hence proposed nanoscale friction models are developed using innovative artificial intelligence-based methods. In fact, although in a previous study the employment of conventional (black box) machine learning methods provided rather good predictive performances, the intrinsic nature of these models prevents their usage in most practical applications. The novel methodology proposed in this work allows, in turn, attaining an extremely simple mathematical formulation (i.e., a white box model) providing an immediate insight and a unique scientific perspective into the multidimensional dependence of nanoscale friction on the studied variable influencing parameters. What is more, this artificial intelligence-based approach allows achieving a high predictive performance with R^2 values in the range of 0.75, while the simplicity of the obtained expressions makes future studies and possible practical applications (e.g. in the corresponding control algorithms) rather straightforward.

Nanoscale friction, artificial intelligence, predictive white box model

1. Introduction

Fundamental physio-chemical phenomena of single-asperity contacts between two contacting surfaces govern the micro- and macroscale frictional behaviour. Friction has, in turn, a negative impact on all precision positioning devices, presenting a major source of stochastic uncertainties. Deepening the knowledge on frictional phenomena at the nanoscale presents, thus, the scientific foundation for the development of novel friction-compensating algorithms, as well as modelling strategies in general [1].

In this work is hence presented the study aimed at modelling nanoscale friction and its dependence on the concurrent effects of three variable process parameters, i.e., normal loading F_N, sliding velocity v and temperature ϑ. The study is performed on thin-film aluminium oxide (Al_2O_3) and molybdenum disulphide (MoS_2) samples synthesized, respectively, via atomic layer deposition (ALD) and pulsed laser deposition (PLD) [2]. With the goal of attaining a mathematical expression that can be used to effectively predict nanoscale friction in the described conditions, data is collected by employing the innovative lateral force microscopy (LFM) based experimental methodology described in [2], thus enabling the training of artificial intelligence (AI) algorithms. Application of AI in this context presents a novel approach adopted progressing from the previously developed black-box machine learning (ML) approach [3].

It will hence be shown that the AI approach, based on using the *TensorFlow* [4] and the SciKit-learn [5] implementations, is a viable method of obtaining compact mathematical expressions that enable describing effectively nanoscale friction from stochastic multidimensional data, while assuring the attainment of high predictive performance metrics values. In fact, the obtained symbolic mathematical expression presents a big step towards identifying the physical laws that underlie the observed complex physical phenomena.

2. AI Numerical Modelling

Evolutionary algorithms are typically used to provide a good approximate solutions to problems that cannot be easily solved using other techniques. The function-generating AI algorithms studied in this frame in this work include age-layered population structure (ALPS), standard Koza style symbolic regression (KS), grammatical evolution (GE) and multi-gene genetic programming (MG).

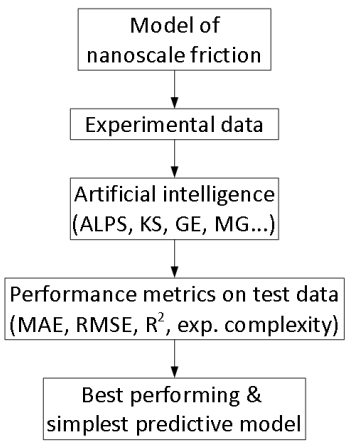


Figure 1. Proposed AI-based methodology of developing the predictive nanoscale friction models

The development of the predictive models is conducted based on the methodology depicted Figure 1. All algorithms are hence trained on 50 values of the measured nanoscale friction forces under the influence of the concurrent multivariate studied process parameters, determined by employing an elaborated design-of-experiments (DoE) methodology, conducted by using centroidal Voronoi tessellation (CVT) sampling [2]. The used experimental data is thus normalized and standardized first. The models are then trained on the set of DoE-CVT-based data [2] for each material separately, as well as on a combined (pooled) dataset for all the considered materials, and then subjected to a 10-fold cross-validation [6]. In the process, an optimization of the hyperparameters of the models is performed [7].

Each developed AI model is then tested for prediction accuracy on a separate test dataset of points unseen during the training of the algorithms, and attained again via elaborated LFM measurements. The test dataset consists of 15 measurement points in the considered multivariate space of process parameters. These points are defined by employing a Monte Carlo (MC) algorithm as implemented in GoSumD software [8]. Contrary to what was done in the case of the DoE-CVD measurements, the data acquisition on the test datased is performed on samples that are not dried prior to the measurements themselves, thus yielding realistic process conditions that provide a more difficult predictive challenge for the used AI numerical models.

Each model's predictive performances are scrutinized therefore on predictions of the nanoscale friction force F_f from the input variables on the test dataset. The metrics used to asses quantitatively each model's predictive performances are the standardised statistical indicators, i.e., the mean absolute error (MAE), the root mean square error (RMSE) and the coefficient of determination (R^2) values [7].

3. Results and Discussion

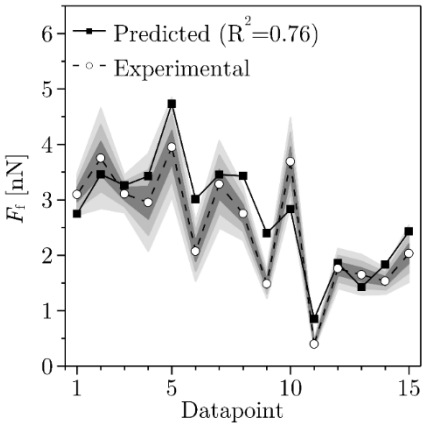
Based on a detailed statistical comparison of the performances of the obtained models it is established that the MG AI algorithm, trained with DoE-CVT-based experimental pooled data, allows attaining the best predictive performance. In fact, the MG result are characterised not only by high R^2 values (Table 1), but enable also achieving relatively compact model expression's length and depth. The hence developed model is therefore use in the following in-depth analyses, i.e., the model is assessed on the test dataset for each of the analysed thin-film sample materials.

Table 1. Performance metrics of the developed MG model

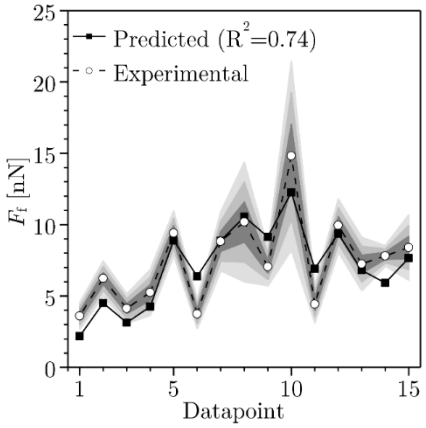
Sample	RMSE	MAE	R^2
Al_2O_3	0.552	0.450	0.760
MoS_2	2.43	2.06	0.736

With the goal of minimizing the developed model's complexity, the selection of the best performing model is then performed by defining a Pareto frontier. The selected best solution allows attaining a regression model characterised by small deviations of the predictions of training and testing data as well as by good stochastic and random properties with good normality.

The results of the performance test of the best-performing MG model on the unseen test dataset is hence shown for the analysed samples in Figure 2. where shaded uncertainty levels present, respectively, the ± σ variance of experimental data (± 1σ as the darkest, ± 2σ as the medium and ± 3σ as the lightest shade of grey). The latter indicates, with empirical near-certainty, all data. Based on the results reported in this figure it can be concluded that the prediction of the nanoscale friction force F_f for both the Al_2O_3 (Fig. 2a) and the MoS_2 (Fig. 2b) sample, next to the relatively high R^2 value, provides also a good fit so that most of predicted nanoscale friction values fall into the ± 3σ uncertainty range of the experimental data.



(a)



(b)

Figure 2. Predictive performances of the best performing MG model on the test dataset for the Al_2O_3 (a) and the MoS_2 (b) sample

Most importantly, the mathematical expressions developed by using the MG algorithm, especially if compared to ML models [3], result in an extremely simple and user-friendly form. Modifying, in fact, the considered load on the samples so as to include the effects of the adhesive forces F_A, so that the total normal load $F_L = F_N + F_A$ is taken into account (see in this regard reference [2]), the dependence of the value of the nanoscale friction force F_f on the concurrent influence of the considered process parameters F_L, v and ϑ, is reduced to respectively, Equation (1) for the Al_2O_3 thin-film, and Equation (2) for the MoS_2 sample.

- for the Al_2O_3 sample:

$$F_f = 0.01183 \cdot F_L - 0.0008751 \cdot v + 0.8707 \cdot \vartheta - 0.0194 \cdot \vartheta^2 + 0.0001258 \cdot \vartheta^3 - 9.67 \quad (1)$$

- and for the MoS2 sample:

$$F_f = 0.04559 \cdot F_L - 0.0008751 \cdot v + 1.751 \cdot \vartheta - 0.02774 \cdot \vartheta^2 + 0.0001258 \cdot \vartheta^3 - 28.41 \quad (2)$$

In these expressions F_L is expressed in nN, v in nm/s, ϑ in °C and the obtained F_f values are given, again, in nN.

To provide a visual representation of the thus obtained dependencies, in Figure 3 are shown the surface plots of the nanoscale friction force F_f values obtained by applying the models of Equations (1) and (2) when two of the process parameters are varied while the third one is kept constant, i.e., when the normal load is F_L = 100 nN, sliding velocity is v = 250

nm/s, and temperature is ϑ = 40 °C. Although these results show a general similarity to the solutions obtained by employing the black box ML models, the solutions obtained via the AI-based approach are much simpler and smoother. What is more, it is evident that for both considered samples the influence of sliding velocity on friction is rather small and smooth, with a negative linear effect vs. temperature. The influence of temperature is, in turn, marked and nonlinear, remaining quite stable when the values of the sliding velocity or of the normal load are varied. Finally, in the right-most column, the effects of sliding velocity and normal load show linear dependences. These results show, therefore, a striking evidence of similarity in the influence of the considered multivariate influencing parameters on the value of the nanoscale friction force F_f. This fact was not only a hard idea to grasp in the earlier stages of this research, especially in the experimental measurement phase, but it is also a result never postulated in the available state-of-the-art.

Based on all the performed tests and evaluations, it can therefore be concluded with a relatively high degree of certainty that, at least for the tested thin-film materials, the developed model realistically reproduces experimental results, but also, importantly, provides a robust and simple predictive tool in establishing the dependence of the value of the nanoscale friction force on the considered variable process parameters F_L, v and ϑ.

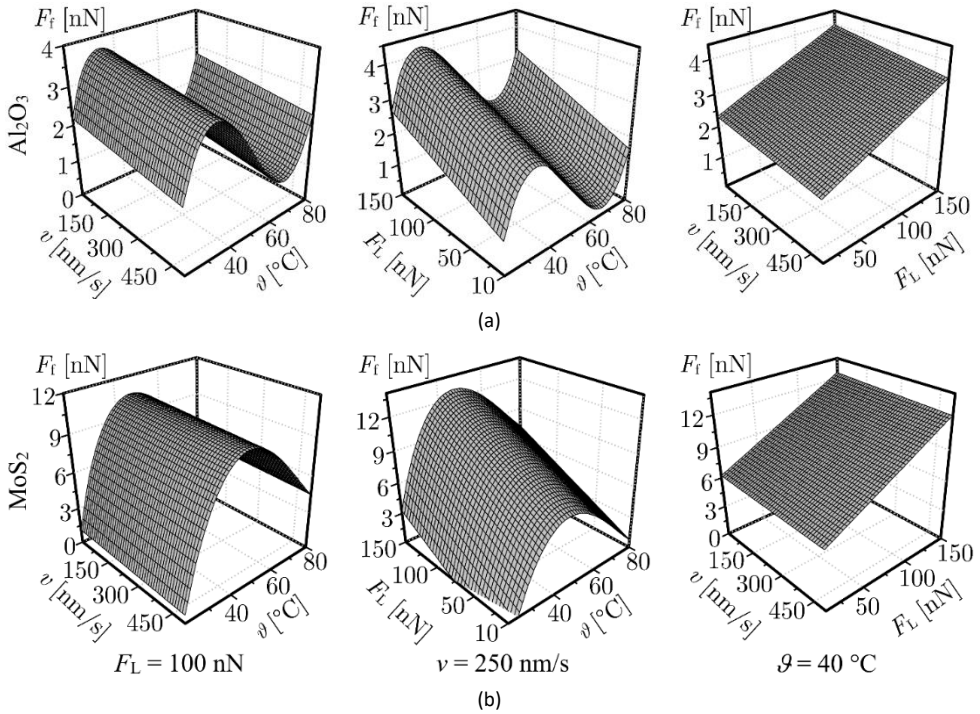


Figure 3. Surface plots of the results obtained via the developed best performing AI-based MG model for constant variables in columns (left to right): total load F_L, v and ϑ, for the Al_2O_3 (a) and the MoS_2 (b) sample

The solutions of Equations (1) and (2) are shown graphically in Figure 4, allowing a visual appreciation of the dependence of the nanoscale friction force F_f on the process parameters for the considered thin-film materials. In the diagrams are visible vertical dashed and dotted lines indicating the limits of the considered variables in the main and unseen test datasets respectively that, considering the fact that the models used to derive the graphs are trained and tested only in these boundaries, provide a sort of safety margin on their validity.

In Fig. 4a is thus shown the dependence of the values of the nanoscale friction force F_f on the total normal load F_L with variable temperatures ϑ and velocities v. It can be seen that, for the considered sample materials, fundamental similarities, with a linear load dependence, emerge, as predicted also by contact mechanics models with adhesion effects. A slight weakening effect of sliding velocity is also evident. The visible diminishing friction with increasing sliding velocities is commonly attributed to the lubricative effect of the water-vapour layer on the surface of the samples. Since the variability of temperature induces a change of the amount of adsorbed water, i.e., a changing state of the meniscus, the adhesive forces also change and so consequently does the total normal load. It can also be noted that for Al_2O_3 a broader scatter between the parallel lines is obtained, i.e., a more pronounced negative dependence is present here.

The influence of sliding velocity v on the F_f value, with variable F_L and ϑ, is depicted in Fig. 4b. These graphs provide a bit more difficult visualization, since there are two strong overlapping effects in the two remaining dimensions. Despite that, it is evident that the influence of v is predominantly small and, as already pointed out, weakening, while the stronger nonlinear influence of temperature induces a change of the absolute value of the velocity effect, but not its trends or strength. The influence of F_L is also evident as a linear shift of the F_f vs. v lines, which induces an increase of the value of the nanoscale friction force.

The already evidenced variability of the influence of temperature ϑ on the value of F_f, with variable F_L and v, is, finally, clear from the distance between the depicted friction lines in Fig. 4c. A larger distance between the curves caused by the change of temperature indicates a clear accentuated temperature effect, which is again well visible on the graph of the Al_2O_3 thin-film sample.

4. Conclusions and Outlook

The usage of novel AI-based methods for the development of experimentally-based predictive models of nanoscale friction is demonstrated in this work.

In contrast to previously developed black-box ML models, the thus developed explicit mathematical expressions are directly understandable and usable, because of their simple mathematical formulation and low number of involved parameters. The analysis of the frictional behaviour in the nanometric domain performed by using the AI algorithms shows, therefore, that it is possible to provide effective predictions of the influence of the multiple process parameter on the value of the friction force with satisfactory levels of accuracy, i.e. high with R^2 values. What is more, the obtained models provide invaluable insight into frictional behaviour of nanoscale frictional contacts with respect to the concurrent influence of three variable process parameters. For both the studied thin-film samples a low diminishing linear effect of sliding velocity, in accordance with conventional friction models, a highly nonlinear effect of temperature, quasi-parabolic for the Al_2O_3 and quasi-sinusoidal for the MoS_2 sample, as well as a linear effect with highly sub-linear characteristic of the total normal load, typical for adhesive contacts, is therefore established and thoroughly examined.

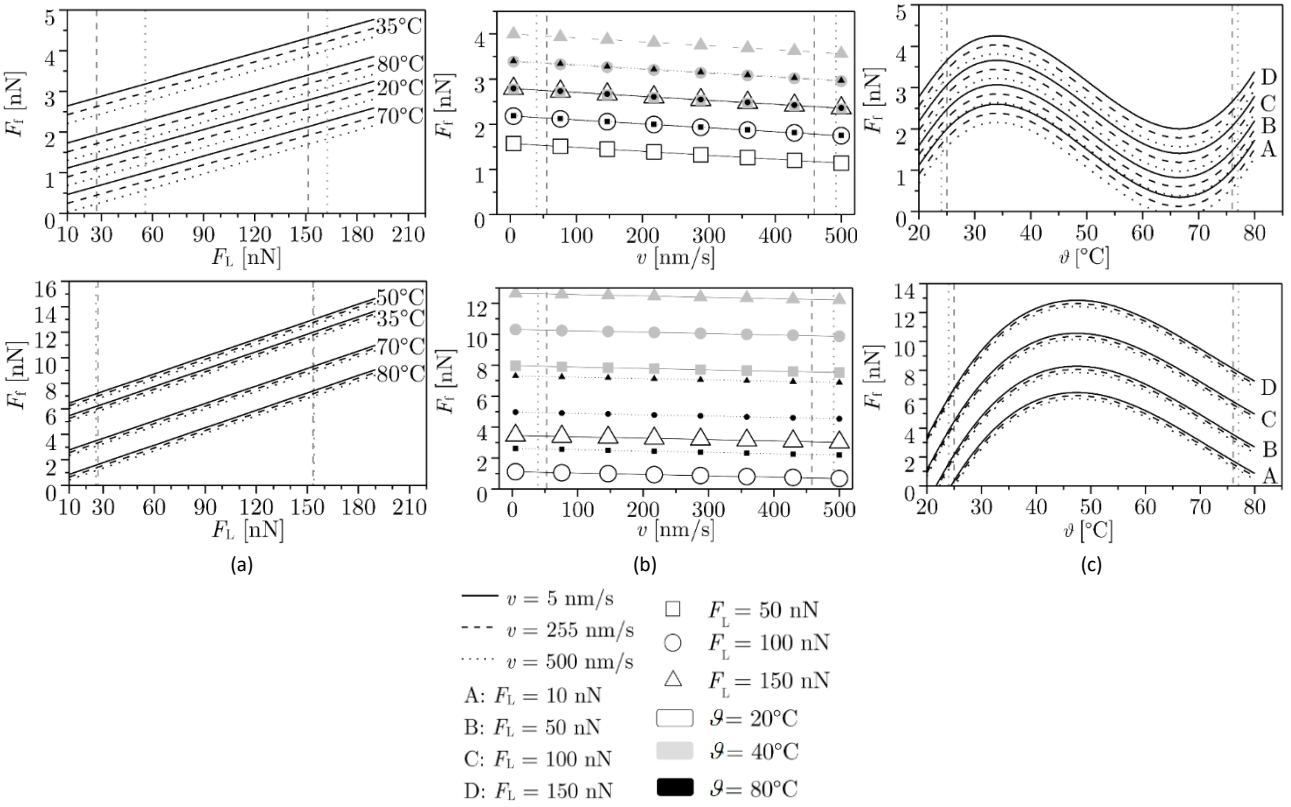


Figure 4. Values of the nanoscale friction force F_f obtained via the developed AI-based MG models vs. the variable parameters: total normal load F_L (a), sliding velocity v (b) and temperature ϑ (c) for the Al_2O_3 (top) and MoS_2 (bottom) sample

All of this provides means for streamlined integration into, modification of, and comparison with existing friction models and numerical schemes, as well as for the direct usage in nanoscale friction prediction, for adaptive control purposes and in further analytical investigations.

The obtained results provide also means for assessing and validating results obtained via molecular dynamics models involving the atomic structures of the surfaces in contact. In fact, further studies in this direction are already underway in collaboration with the Molecular Biology and Nanotechnology Laboratory (MolBNL) of the University of Trieste, Italy [9].

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