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A molecular dynamics study of nanometric scale friction

Marko Perčić,[1, 2, 3] Andrea Mio,[4] Saša Zelenika [1, 2, 3] and Maurizio Fermeglia [4]

[1] *University of Rijeka, Faculty of Engineering, Precision Engineering Laboratory, Vukovarska 58, 51000 Rijeka, CROATIA*
[2] *University of Rijeka, Centre for Micro- and Nanosciences and Technologies, Laboratory for Precision Engineering and the Micro- and Nanosystems Technologies, Radmile Matejčić 2, 51000 Rijeka, CROATIA*
[3] *University of Rijeka, Centre for Artificial Intelligence and Cybersecurity, Laboratory for AI in Mechatronics, Radmile Matejčić 2, 51000 Rijeka, CROATIA*
[4] *University of Trieste, Department of Engineering and Architecture, Molecular Biology and Nanotechnology Laboratory (MolBNL), Piazzale Europa 1, 34127 Trieste, ITALY*

sasa.zelenika@riteh.hr

Abstract

Friction is an omnipresent phenomenon in all mechanical systems, inducing uncertainties and acting as a major disturbance in manufacturing technologies and in the field of the micro- and nanoelectromechanical systems (MEMS & NEMS). The effects of friction can generally be compensated in the macro- and mesoscale applications. Multiple concurrent effects of various atomic-scale phenomena in the asperity contacts hinder, however, the prospect of a satisfactory insight into the fundamental tribological behaviour in the micro- and nanoscales. An in-depth fundamental understanding of nanoscale frictional behaviour is, thus, of outmost technological importance. An approach using molecular dynamics (MD) simulations is, hence, proposed in this work to study the tribological behaviour in the nanoscale (atomic) contacts. Recent thorough scanning probe microscopy experimental measurements of nanoscale friction on various thin-film materials are thus used as benchmark for MD simulations, allowing to attain important insights into the dynamics of a sliding tip on an aluminium thin-film surface while varying the normal loads. A sound basis for future more complex models, which will include adhesive effects and oxide layers, is thus accomplished, creating the preconditions to deepen further the fundamental knowledge of important tribological phenomena.

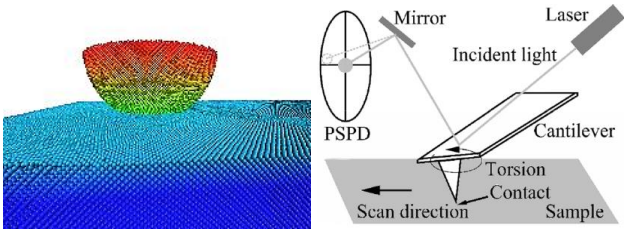
Nanoscale friction, molecular dynamics, atomistic simulation

1. Introduction

Frictional phenomena have a detrimental effect in precision manufacturing and in the field of the micro- and nanoelectromechanical systems (MEMS & NEMS). On the other, hand, friction with its marked stochastic behaviour is still insufficiently studied at the fundamental level. In fact, to gain fundamental insights on frictional phenomena, particularly for complex nanostructured materials, it is crucial to study the physical and chemical origins of friction. Multivariate concurrent effects occurring in the nanometric contacts are, in turn, governed by atomic interactions between the asperities of the surfaces of bodies in relative motion [1]. These can be idealized as atomistic structures with interaction potentials using molecular dynamics (MD) methods. An approach involving MD atomistic modelling is proposed in this work as means of investigating the frictional characteristics of single-asperity contacts. The simulations are calibrated and benchmarked to recent experimental data on nanoscale friction between a silicon (Si) tip of a Bruker Dimension Icon scanning probe microscope (SPM) and an aluminum (Al) thin film sample, obtained in contact-mode lateral force microscopy (LFM) measurements [2].

2. Materials and methods

Due to their moderate cost, low entry barriers, rapidity, versatility and a tight process control, in the last couple of decades *in silico* techniques of investigating nanotribological properties play a crucial role in materials science [3]. The computational methods employed nowadays for studying nanotribological phenomena comprise different techniques, from the mentioned MD approach, to Monte-Carlo (MC) simulations and density functional theory (DFT) based methods. The use of MD atomistic models is particularly extensive by virtue of their high temporal and spatial resolution, making them suitable for reproducing and widening the results of experiments aimed at establishing the mechanical properties of solids, attained by using measurement methods such as SPM, nanoindentation, nanoscratching, wear tests, etc. (Fig. 1a).



(a) (b)

Figure 1. Atomistic MD simulations (a) and corresponding LFM measurements (b).

The experimental LFM methodology is based, in turn, on an Si tip in continuous sliding contact with a sample surface (Fig. 1b). In fact, recent LFM experimental measurements [2], processed by using state-of-the-art machine learning (ML) based methods, enable obtaining the predictive functional dependencies of the influence of the multivariate concurrent technological parameters on the nanoscale friction forces [4]. The thus modelled data can hence be used to extrapolate the dependency of the nanometric friction force on the values of the normal loads. A set of MD simulations on an atomistic model of the SPM tip in contact with an Al thin-film surface, mimicking the performed LFM test,

is therefore carried on with the aim of exploring and comparing the behaviour of the studied tribological configuration at different normal loads ranging from 7 nN to 1 090 nN.

The developed MD dynamical model comprises an Si tip placed above a single crystalline Al surface, which is outside the interaction range of the interatomic potentials. The indenter tip apex is modelled by placing the Si atoms within a hemispheric region with a lattice constant of 5.43 Å. The radius of the indenter tip comprises 20 unit cells, i.e., it is about 10.86 nm, and it contains 135 289 atoms. The workpiece is, in turn, structured as a face-centred-cubic (FCC) region with a lattice constant of 4.05 Å and a lattice orientation of [100], [010] and [001] along the x, y and z axis, respectively. The sample surface is $100 \cdot a$ x $250 \cdot a$ x $25 \cdot a$, where a is the lattice constant of Al, thus corresponding to a 40.46 x 101.15 x 10.12 nm^3 workpiece containing about 2.5 million atoms. Both structures are composed of three atomic layers, each fulfilling a different need. The boundary atoms are preventing the sliding motion of the system, the Nosè-Hoover thermostat atoms are used for keeping the vibrations of the atoms within a realistic range, while the Newtonian atoms are free of constraints and move under the load of the interatomic and applied forces. To provide a reliable MD simulation, the definition of an appropriate forcefield is non-trivial. As suggested in prior art [5-6], a multibody modified embedded-atom method (MEAM) forcefield [7] is thus employed for the definition of the interatomic interactions within each material, while the respective parameters are set as proposed in [8]. The interaction between the atoms of different materials is, in turn, determined by using the 12-6 Lennard-Jones (LJ) potential energy, based on the Lorentz-Berthelot mixing rules [9]. As done previously for a similar system [10], the LJ potential cut-off distance is set at $2.5 \cdot \sigma$, where σ is the equilibrium distance influencing the potential energy of a pair of atoms. To reveal distinctly the sub-nanoscale frictional behaviour, the possible presence of the oxidation of the Al workpiece and the Si tip surfaces, or of a water-vapour layer, is neglected in these MD simulations.

The simulations are then structured in four steps. The system is created first and fully relaxed (equilibrated) at 300 K. The application of the normal load on the boundary atoms of the tip is then performed to establish the contact of the tip apex with the workpiece and the indentation into it. As soon as the tip reaches the desired indentation, load is removed and the system is relaxed once more to assure a stable 300 K temperature value. A lateral velocity of 0.5 nm/ps in the [010] direction is finally applied to the tip, performing several scratching motions along the (001) plane of the surface of the Al thin-film sample.

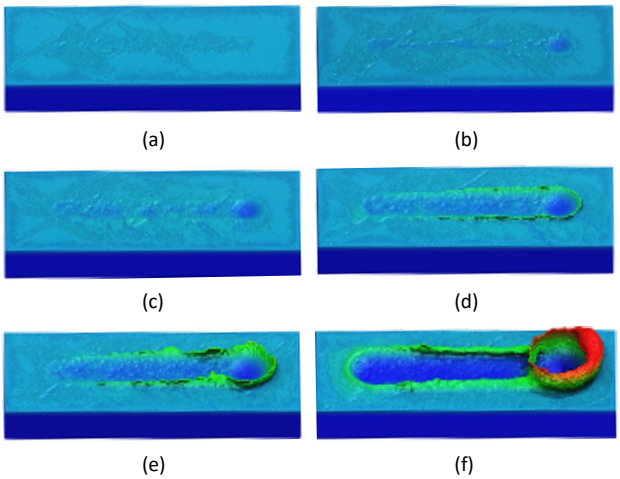


Figure 2: Evolution of sliding contacts on the Al sample for rising loads: 7 nN (a), 274 nN (b), 427 nN (c), 650 nN (d), 724 nN (e) and 1 090 nN (f).

3. Results and discussion

The results of the MD simulations for increasing loads, focused on the Al surface, are shown in Fig.2, where the pile-up of the atoms in the sliding direction can be clearly noted for higher normal loads. Results obtained by extrapolating the predictions of the ML models, developed based on the LFM experimental data, and of the performed MD simulations, are, in turn, compared in Fig. 3. The graph depicted in this figure shows a clear linear dependency of the value of the nanoscale friction force F_f on the normal load F_N obtained from the ML model. Although a similar trend is obtained also via the MD simulations, in this case a slight nonlinearity appears. It could be speculated that this effect is induced by the pile-up resistance in the MD model, evident especially for loads above 600 nN, when a noticeable rise of F_f is induced (cf. in this regard again Fig. 2).

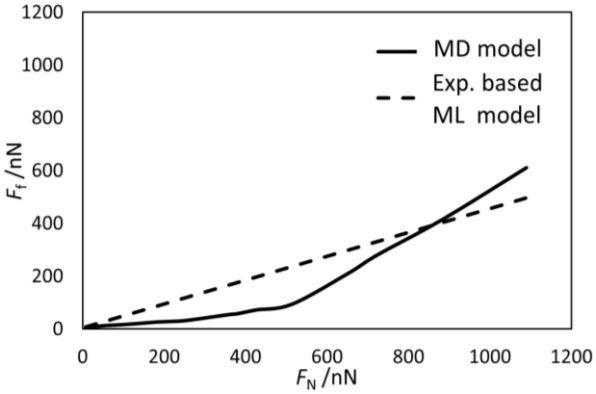


Figure 3. Comparison of F_f values obtained from ML and MD simulations.

4. Conclusions

An MD-based approach to modelling nanoscale friction is presented in this work. The thus obtained results are compared to those of the ML model based on LFM measurements performed on an Al thin-film sample. Bearing in mind the inevitable extrapolation errors of experimentally-based ML models, as well as the spatio-temporal limitations of the MD methods, the results show remarkable similarities in trends, providing important insights in the fundamental principles governing nanoscale tribological phenomena. The performed simulations provide a solid basis for advanced studies with models that could also include complex phenomena induced by adhesion, the oxide layers, or the presence of water-vapour molecules at the sliding interface, thus creating the preconditions for advancing further the fundamental knowledge on nanoscale friction.

Acknowledgements

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