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A Molecular Dynamics approach to investigate the tribological behaviour of Al-Si and α-Al_2O_3-Si interfaces at the nanoscale

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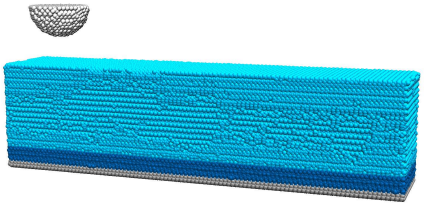
Introduction

The evolution of Information and Communications Technology (ICT) and Micro-Nano Electromechanical System (MEMS/NEMS) makes evident the trend towards the **progressive miniaturisation** of devices. The **energy efficiencies** at the nanoscale are, in turn, significantly lowered by **friction force**. The friction force depends not only on the **tribological pair parameters** and **normal loads**, but also on **the crystalline structure** of the materials in contact, their **surface chemistry** and **roughness**. Our research focuses on the nanometric friction force using **Molecular Dynamics (MD)** simulations. An investigation of a system comprising a **hemispheric silicon tip** sliding on an **aluminium oxide** flat surface, aiming at understanding the interactions between the materials from an atomistic standpoint, was thus conducted.

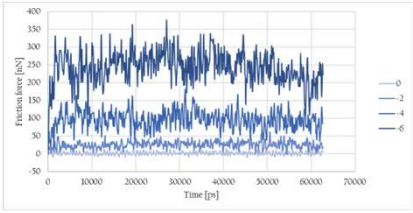
Materials and Methods

The large dimensions of the simulated system **(400,000 atoms, tip diameter≈25 nm)** required the usage of the HPC capacities available at the **"Bura"** facility of the University of Rijeka, Croatia. The materials have thus been simulated using **LAMMPS** following a modelling procedure via **four** subsequent steps: initially, the tip/surface system was generated, with an appropriate hybrid force field **(comb3** and **Lennard-Jones)**. The surface was composed by **three atom layers**, each one fulfilling a different need: boundary atoms, thermostat atoms and Newtonian atoms. The first layer of unit cells located on the bottommost facet of the aluminium oxide workpiece were kept fixed in space as **boundary atoms** (grey coloured). They were built to **prevent** the surface from being subjected to **translational motion** during the indentation phase. The atoms belonging to several consecutive parallel layers of unit cells adjacent to the bottommost boundary atoms (15 nm), shown in blue, were subjected to a **barostat** at **1 atm** and **thermostat**, at a constant temperature of **300 K**, simulating the heat dissipation in the real LFM test. The remaining atoms (light blue coloured) were **free of constraints** and moved according to interatomic and applied forces. Then, to induce the contact between the tip and aluminium oxide surface, the rigid tip was subjected to a **normal load.** While the tip was moving downwards, **various indentation depth** have been set and used as a starting point for the following scratching phase. Lastly, **lateral velocity** was applied to the tip, exploring the influence of **different indentation depths**. The simulation **outcomes** were **compared** to highlight their advantages and drawbacks in terms of the modelling of realistic tribological systems.



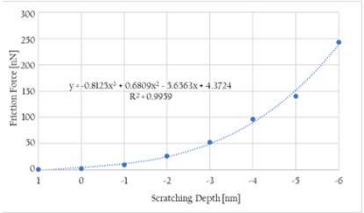
Results and Discussion

Friction force as function of the scratching length for different scratching depths at a constant sliding velocity

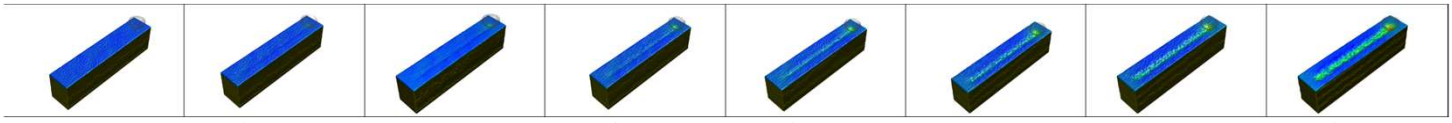


The friction force is almost constant during the overall sliding distance, with a little increase at the beginning of the scratching phase due to the need to overcome the static friction force. High frequency noise is due to generation and breakage of weak bonds.

Friction force as function of the scratching depth at a constant sliding velocity



The proposed polynomial model can accurately predict the trend of the friction force. The friction force increases exponentially with the scratching depth, according to the increment of the bonds generated between tip and workpiece. This model can be used to interpolate the friction force for low scratching depths.



1 nm | 0 nm | -1 nm | -2 nm | -3 nm | -4 nm | -5 nm | -6 nm

The workpiece exhibits an evident trace due to the sliding of the tip for scratching depths larger than 3nm. Experimental tests are underway to validate the outcomes gained through *in-silico* modelling. The performed simulations provide a solid base for advanced studies with models that could also include complex phenomena induced by adhesion, or the presence of water-vapour molecules at the sliding interface, thus creating the preconditions for advancing further the fundamental knowledge on nanoscale friction.

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