## **Division of Mechanics**

## Friction mechanisms during the contact and sliding process modelled by MD simulations Master theses 30hp

Friction is one of the oldest phenomenon studied in natural sciences. In a macroscopic scale it is known that the friction force between surfaces satisfies the following rules: (1) The friction is independent of contact area between surfaces; (2)It is proportional to the normal force applied between surfaces and (3) The kinetic friction force is independent of relative speed between surfaces[1]. Considering that friction is the result of many microscopic interactions between the building atoms at the surfaces, it must depend on factors as roughness, temperature and the energy dissipation mechanism at the surfaces. Therefore, to understand its macroscopic behavior it is necessary to understand in details the dynamics of interaction between atoms in the surfaces in contact. The proposed Master project aims at investigating the mechanisms of friction phenomena at nanoscale based on molecular dynamics (MD). Simulation will be performed using the free software LAMMPS. In the first part of the Master thesis a MD model will be developed and different aspect of the friction mechanics will be studied.



The second part of this work will focus on correlating the simulation results with experiments from scratch tests. Deformation patterns obtained in the simulations will also be directly compared to the traces of slip activity on polished specimen surfaces in the experimental findings.

The work is suitable for 2 students and can start in January 2021.

Contact: Prof. Aylin Ahadi, Division of Mechanics, <u>aylin.ahadi@mek.lth.se</u> Prof. Dmytro Orlov, Division of materials engineering, <u>dmytro.orlov@material.lth.se</u>

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