Computational Chemistry applied to Tribology: a Molybdenum Disulfide case study

Paolo Nicolini

Department of Control Engineering - K335, Faculty of Electrical Engineering
Czech Technical University in Prague, Czech Republic

One third of energy produced by industrial countries is lost as friction. High wear caused by friction means that ca. 35% of the industrial production is used to replace degraded products, whilst causing the breakdown of machinery, resulting in safety risks and environmental pollution. Controlling and reducing friction is a fundamental step in attaining the sustainable development of our society, as detailed in the Brundtland report. In this seminar, I will first briefly introduce the topic, and then I will present two recent studies that we performed on molybdenum disulfide, a widely used solid lubricant.

In the first study, by means of molecular dynamics (MD) simulations and exploiting a reactive classical force field, we investigated the shear induced structural changes and possible layer formation in amorphous molybdenum disulfide. The ordering process is studied in details, with particular regard to the estimation of the thermodynamic properties that govern the process itself. A connection with the framework of classical nucleation theory was also found, conferring a predictive power to the achieved results. Overall, this study aims at gaining an atomic level understanding of the dynamics of layer formation process in molybdenum disulfide, thus controlling and possibly improving its tribological properties.

The second study is focused on the sliding dynamics of molybdenum disulfide against itself at nanoscale, both from the experimental and from the computational points of view. The differences between ordered material (single crystal) and disordered material (sputtered coating) were investigated. Tribological experiments were performed using atomic force microscopy (AFM) exploiting the lateral force measurement mode. AFM tips modified by sputter deposition of molybdenum disulfide were used for the first time. This feature opened up the possibility for close comparison with classical MD simulations. In both cases, the coefficient of friction for the ordered system in inert conditions was found to be smaller than for disordered system. This result demonstrates the impact of morphology at the nanoscale and highlights the importance of MD as a diagnostic and predictive tool in nano-friction. These findings can expedite the process of fabricating molybdenum disulfide-based coatings with superior tribological properties, with the ultimate aim of reducing the energy dissipation due to friction.

References

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