PRESS RELEASE

ERC Advanced Grant for Michael Moseler from the Fraunhofer IWM: Digital twin for lubricants in highly loaded tribological contacts

Prof. Dr. Michael Moseler, Head of the Tribology Business Unit at the Fraunhofer Institute for Mechanics of Materials IWM in Freiburg and Professor for Simulation of Functional Nanosystems at the University of Freiburg, has been awarded an ERC Advanced Grant worth 2.5 million euros for the research and development of a digital twin that can describe lubrication under high loads and thus predict the design and operating conditions for energy-efficient machines. An ERC grant is one of the most prestigious awards in European research funding and is awarded to top researchers for outstanding scientific research approaches.

Friction is everywhere. Wherever components move against each other, energy is consumed. Globally, friction accounts for up to 20% of energy use – despite many technological solutions aimed at reducing it, such as new lubricants and coatings.

Michael Moseler aims to show how this untapped potential for energy savings and sustainability can be unlocked by developing a digital twin for lubricated frictional contacts. To realize this ambitious research project, he is receiving an ERC Advanced Grant worth 2.5 million euros over a period of five years from the European Research Council.

The challenge lies in making friction-inducing processes in technical systems—processes that occur on the atomic level and are inaccessible to experiments—computationally predictable. These include, for example, viscosity changes in lubricants within nanoscale frictional gaps or the sliding of solidified lubricant films over material surfaces.

To this end, a novel approach using computer simulations is employed. Simulation methods and calculation models that describe the mechanisms on the different scales, are combined into a single tool to capture the friction-inducing features and predict the behavior of the tribological system. Once the causal relationships between atomic-scale processes and energy-consuming friction are mathematically described for a given technical system, the system can be optimized.

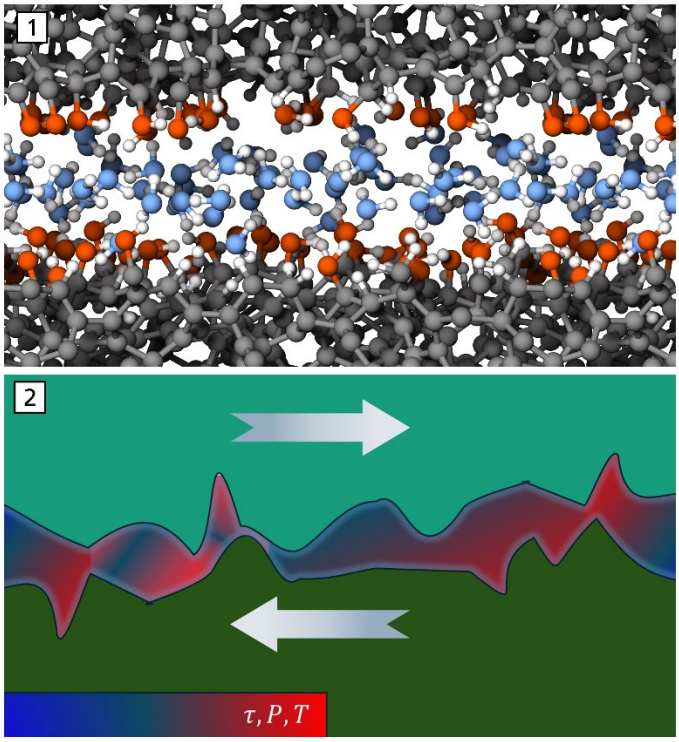
Extreme-scale molecular dynamics simulations will be used to capture the atomic effects in the friction zone. A key aspect of the project is the development of physics-

Press Contact
Thomas Götz | Telefon +49 761 5142-153 | thomas.goetz@iwm.fraunhofer.de
Scientific Contact
Prof. Dr. Michael Moseler | Telefon +49 761 5142-332 | michael.moseler@iwm.fraunhofer.de
Fraunhofer Institute for Mechanics of Materials IWM | Wöhlerstrasse 11 | 79108 Freiburg | www.iwm.fraunhofer.de

based material models that accurately reflect the behavior observed in molecular dynamics. For instance, precise constitutive equations must be determined for the rheology and tribochemical reactions of lubricant films just a few nanometers thick under gigapascal pressures. These will be integrated into continuum equations and will form the core of the digital twin, which aims to model thermo-elasto-hydrodynamic lubrication in highly loaded components (such as rolling bearings and gear contacts). The project will use automated workflows for high-throughput molecular simulations of frictional contacts under a wide range of load parameters. In addition, it will employ the latest generation of machine-learning interatomic potentials (MLIPs), which offer quantum-mechanical accuracy at a fraction of the computational cost.

What makes this research approach unique is the combination of extremely large-scale atomistic simulations, machine-trained AI force fields, and the integration of the resulting physical constitutive equations into a continuum description of the highly loaded lubricant. This allows for virtual insights into previously inaccessible friction mechanisms. Further success factors include the intelligent and efficient use of massive computing resources—simulating up to one billion atoms—and the development of a powerful digital infrastructure for managing the resulting data streams and data analyses.

Within five years, this digital twin is expected to bridge the gap between atomic friction phenomena and the design of bearings and gearboxes, contributing to greater sustainability and energy efficiency in machines, devices, and vehicles.



The digital twin for lubricants in highly loaded frictional contacts establishes a mathematical link between the atomic dynamics in the lubrication gap and macroscopic friction. With an understanding of the fundamental causes of the friction-related energy consumption of technical systems such as bearings and drives, it becomes possible to design more energy-efficient machines, plants and vehicles.

Fig. 1: Molecular dynamics simulation of a glycerol-lubricated frictional contact between two diamond-like carbon layers under high mechanical load. Such tribological systems can be used, for instance, to build novel superlubricated plain bearings. The molecular dynamics simulation provides material laws for the lubricant behavior.

These, in turn, are used in higher-scale fluid dynamics simulations of lubricated rough surfaces to predict macroscopic friction (Fig. 2).

Fig.: Prof. Dr. Michael Moseler, © Fraunhofer IWM, Photo: Kai Wudtke

About Michael Moseler

Prof. Dr. Michael Moseler is a German physicist and materials scientist with a strong focus on atomistic modeling of friction, lubrication, and wear. He heads the "Tribology" business unit at the Fraunhofer Institute for Mechanics of Materials IWM and holds a professorship for "Simulation of Functional Nanosystems" at the Department of Physics at the University of Freiburg. His research includes classical and quantum-mechanical molecular dynamics simulations of tribologically induced phase transitions, the rheology and reactivity of lubricants under strong confinement as well as fundamental mechanisms underlying superlubricity. In 2022, Moseler received the prestigious Stifterverband Science Award for his "Virtual Material Probe for Tribological Contacts" (see https://youtu.be/c75_Z7WdHms).

Funding Statement

The development of a digital twin for lubricants in highly loaded tribological contacts is being funded by the European Union as part of an "ERC Advanced Grant". ERC-2024-ADG, Project 101201061 – LubeTwin.

The **Fraunhofer IWM** is passionate about sustainability in industrial value creation. Through its research and development work, it opens up new pathways and design opportunities for durability and safety in components, resource efficiency in process chains, and energy efficiency in machines. The institute makes materials within process chains, components, and machines predictable in terms of their behavior and properties. It investigates the effects of mechanical, tribological, thermal, electrical, and chemical stresses on the function and durability of materials and develops solutions that allow these materials to be used as adjustable systems in processes and components.

The **Fraunhofer-Gesellschaft** based in Germany is the world's leading applied research organization. Prioritizing key future-relevant technologies and commercializing its findings in business and industry, it plays a major role in the innovation process. A trailblazer and trendsetter in innovative developments and research excellence, it is helping shape our society and our future. Founded in 1949, the Fraunhofer-Gesellschaft currently operates 76 institutes and research units throughout Germany. Over 30,000 employees, predominantly scientists and engineers, work with an annual research budget of €2.9 billion. Fraunhofer generates €2.5 billion of this from contract research.