2023 Helmholtz – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

PART A

Title of the project:

Employing machine learning to identify critical surface topography features

Helmholtz Centre and/or institute:

Karlsruhe Institute of Technology (KIT)

Project leader:

Prof. Dr. Christian Greiner

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Description of the project (max. 1 page)**:**

Almost 25 % of mankind's primary energy usage can be traced back to friction and wear. It is therefore tribology – the science of friction, wear and lubrication – that holds extreme promise when it comes to reducing mankind's CO_2 emissions. To realize this potential however, first we need to develop the ability to predict and control friction and wear. This is currently not possible as a comprehensive understanding of tribological properties has so far been out of reach, even after decades of fundamental tribological research. This is – in part – due to the complexity of any tribological system, which is influenced and controlled by a wide range of factors, including the microstructure of the materials making up the contact [1,2], the surrounding medium and the environment [3], as well as the topographies of the two contacting bodies [4,5]. In order to characterize the latter, currently surface profile measurements mainly rely on simple scalar

quantities such as roughness and waviness values like R_a and W_t. These scalars however are by no means able to represent the complexity inherent to every technical surface [6]. It is therefore currently not possible to conclusively correlate surface topography with tribological properties. This in turn means that there is a huge potential to tailor – and minimize – friction and wear once such a correlation has been established and guidelines can be given what kind of a surface topography should be the result of a production process for a desired set of tribological properties. Not too long ago, aiming at such a correlation would have been impossible. Today however, with the advent of sufficiently powerful and accurate machine learning tools, this can and should be embarked on [7]. Consequently, this is exactly the challenge we are setting for this proposal as we are convinced it truly is a "grand challenge" and therefore extremely suitable for Helmholtz research. We will do so by gathering high-quality surface topography and tribological data. This is possible in Prof. Greiner's lab as here several tribometers have been set-up which can gather data with up to the MHz regime and all relevant metadata and data is automatically stored in an electronic lab book system. This system also allows for a fast and efficient analysis of the data. The same goes for the topography data which is for example measured by white light or confocal microscopy as well as by atomic force microscopy.
The main objectives of our research are:
1. Gather sufficient and high quality tribological data from various tribometers.
2. Employ a machine learning-based framework for surface topography analysis in tribology using existing datasets. We might also involve simulation data, if time permits.
3. Apply the developed framework to correlate surface topography with tribological properties.
4. Test this correlation by tailoring tribological behaviour through manufacturing customized surface topographies.

References:
[1] Haug C. et al. "Tribologically induced crystal rotation kinematics revealed by electron backscatter diffraction. “ Acta Materialia, 2022.
[2] Pastewka L. et al. "Anisotropic mechanical amorphization drives wear in diamond." Nat Mater, 2011.
[3] Schreiber PJ. et al. "Liquid superlubricity obtained for self-mated silicon carbide in nonaqueous low-viscosity fluid." Tribology International, 2019.
[4] Aghababaei R. et al. “Asperity-Level Origins of Transition from Mild to Severe Wear.” Phys Rev Lett, 2018.
[5] Meine K. et al. "The influence of roughness on friction." Wear, 2002.
[6] Jacobs T. et al. "Quantitative characterization of surface topography using spectral analysis." Surf. Topogr., 2017.
[7] Max M. et al. "Current Trends and Applications of Machine Learning in Tribology—A Review." Lubricants, 2023.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

Name: Prof. Dr. Linmao Qian
Institute: School of Mechanical Engineering, Southwest Jiaotong University
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Professor Qian is a full professor and serves as the dean of the School of Mechanical Engineering at Southwest Jiaotong University, which is recognized as a top-tier university under the Double First

Class University Plan and former Project 211. His research involves materials tribology and surface engineering as keys to developing materials tailored for specific tribological applications allowing for lower frictional energy dissipation and longer component lifetime.

Recently, our research group has established preliminary contacts and engaged in academic discussions with Professor Qian's team. We are delighted to find that our research directions are highly complementary, and our future scientific research plans significantly share commonalities, indicating a promising prospect for in-depth collaboration. The current OCPC project marks an excellent beginning for a long-term cooperation.

Our respective experimental teams have conducted in-depth research on surface topography and materials tribology. Within Professor Qian's group, research emphasizes nanoscale topography and material properties, whereas Professor Greiner's group focuses on micro and meso length scales. At the same time, the KIT lab has significantly more expertise in machine learning and the use of electronic lab notebooks as well as generating FAIR experiments. These strengths enable us to engage in multi-scale tribology research, which will help to fulfil the long-standing goal of predicting and controlling tribological behaviour.

Required qualification of the postdoc:

- Ph.D. in Mechanical Engineering or Material Science
- Experience with Tribology
- Additional skills in surface topography and machine learning
- Language requirement: very good written and spoken English

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