# An atomistic study of temperature and surface chemistry effects on the slip constitutive law of polyalfaolefins in contact with amorphous carbon

Stefan Peeters*†[1], Edder J. Garcia[1,2], Franziska Stief[1,3], Kerstin Falk[1], Gianpietro Moras[1], and Michael Moseler‡[1,2,3]

[1]Fraunhofer IWM, MicroTribology Center TC, Freiburg, Germany – Germany
[2]Freiburg Materials Research Center, University of Freiburg, Germany – Germany
[3]Institute of Physics, University of Freiburg, Germany – Germany

**Abstract**

The quantitative description of lubricants in nanoscale channels is complicated by various effects that are often neglected in conventional elastohydrodynamic models. One of those effects is wall slip, a phenomenon that has been extensively studied both theoretically and experimentally. Slip occurs whenever the velocity of a solid wall and the fluid in contact with the wall differ, changing the shear rate of the fluid, thus the shear stress, with respect to the no-slip condition. There is evidence for friction reduction in the elastohydrodynamic regime due to slip (1), which is connected to the limited momentum transfer, i.e., energy dissipation, between the lubricant molecules and the surface of the wall (2). However, some authors suggest that thermal effects, which change the viscosity of the fluid, are responsible for low friction (3). Slip depends on a variety of different properties of the system, ranging from the pressure, temperature and shear stress in the lubricant, to the surface chemistry and the commensurability between lubricant molecules and the surfaces. Due to the relevance of slip especially at the boundary lubrication regime, we performed an extensive molecular dynamics study on the effect of temperature on the slip of a polyalphaolefin base oil in a nanosized amorphous carbon channel. We observed that higher temperatures promote the slip of the lubricant molecules on the surfaces, changing the parameters of the Eyring constitutive law (4), which describes slip as an activated process. The emergence of an interfacial thermal resistance is connected to slip since both effects originate from the incommensurability between lubricant and wall. Nonetheless, we show that temperature effects have a limited impact on the viscosity of this lubricant, and therefore we argue that low friction mainly comes from slip. These results represent a first step towards the definition of a non-isothermal slip law to extend the validity of continuum models for lubrication. We will also discuss our preliminary results regarding the effect of the surface chemistry, particularly the surface termination of amorphous carbon, on the slip properties of the lubricant.

(1) M. Kalin, Tribol. Online 7, 3, 112 (2012)
(2) R. Khare et al, Int. J. Heat Mass Transf., 49, 19-20, 3401 (2006)
(3) M. Björling et al., Tribol. Lett. 55, 2, 353 (2014)
(4) F.-C. Wang, Y.-P. Zhao, Soft Matter 7, 18, 8628 (2011)

*Speaker
†Corresponding author: stefan.peeters@iwm.fraunhofer.de
‡Corresponding author: michael.moseler@iwm.fraunhofer.de