MM 38: Invited talk Pastewka

Time: Wednesday 15:00-15:30

Location: H38

Invited Talk MM 38.1 Wed 15:00 H38 Models for adhesion, friction and wear across the scales — •LARS PASTEWKA¹, PETER GUMBSCH^{1,2}, MICHAEL MOSELER², GIANPIETRO MORAS², ANKE PEGUIRON², and MARK ROBBINS³ — ¹Karlsruhe Institute of Technology, Institute for Applied Materials, Karlsruhe, Germany — ²Fraunhofer IWM, Freiburg, Germany — ³Department of Physics and Astronomy, Johns Hopkins University, Baltimore, MD, USA

Adhesion, friction and wear are processes where the surface of a material plays a central role. Studying these processes is made complicated by most surfaces rough topography, their interaction with the environment, and the inaccessibility of the interface between two materials to *in situ* experimental techniques. In this talk, I give examples of how computer simulations at mesoscopic to atomic scales can help to elucidate the processes that take place at these buried interfaces. Mesoscopic simulations of elastic contact between randomly rough surfaces allow a direct calculation of the area of intimate atomic contact and reveal emergence of macroscopic adhesion as a function of topography and microscopic surface forces. Conditions within the contacting regions are typically extreme and give rise to severe plastic deformation and change of the material microstructure. Atomic-scale calculations based on classical molecular dynamics, tight-binding and density-functional theory under such conditions reveal how this "tribomutation" evolves in diamond and amorphous carbon, and how its formation facilitates wear of these materials in contact with each other and in contact with oxide ceramics.