

Plenary Talk

PV XII Thu 18:00 H1

Making and Breaking of Atomic Bonds in Carbon Tribocontacts — ●PETER GUMBSCH^{1,2}, MICHAEL MOSELER¹, and LARS PASTEWKA¹ — ¹Fraunhofer IWM, Freiburg, Germany — ²KIT, Karlsruhe, Germany

Modelling of tribological contacts, of friction and wear processes, has to cover many orders of magnitude in length and time scales from the atomic scale to the size and lifetime of engineering components. Atomistic processes are obviously crucial for the mechanics of the contacts which in turn determine the wear processes that limit the lifetime of machining components. The physics-based modelling and simulation

of friction and wear processes is still in its infancy. I will describe first atomistic approaches to the simulation of tribocontacts between diamond surfaces and diamond-like carbon (DLC) films. Different levels of approximations are required to assess the evolution of the friction contacts. Considerable attention must be paid there to extracting relevant information from large scale atomistic simulations, which in turn first requires an atomistic model for the hydrocarbons that can describe well the making and breaking of the atomic bonds. I will present results for the evolution of an atomically determined friction coefficient during running-in of such a contact and will later turn to the question of how the polishing of diamond proceeds.