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Making and Breaking of Atomic Bonds in Carbon Tribocontacts

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Friction and wear are particularly illustrating examples of the multitude of length and time scales that are relevant in the mechanics of materials. Any modelling has to span from the atomic scale to the size and lifetime of engineering components. Atomistic bond breaking processes and picosecond time scales are obviously crucial for the wear processes which in the long run determine the lifetime of machining components. Partly due to the difficulty in bridging all these length and time scale, the physics-based modelling and simulation of friction and wear processes is still in its infancy. I will describe our first atomistic approaches to the simulation of tribocontacts between diamond-like carbon (DLC) films or diamond. Different levels of approximations are required to assess the evolution of the friction contacts. Considerable attention must be paid 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 atomistically determined friction coefficient during running-in of such a contact and will later turn to the question of how wear processes and the polishing of diamond proceed.