

Plenary Lecture



Professor Peter Gumbsch

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Title: Making and Breaking of Chemical Bonds

Materials modelling covers many orders of magnitude in length and time scales. Modelling has to span from the atomic scale to the size and lifetime of engineering components. A particularly illustrating example where this multitude of scales is of obvious importance is the catastrophic failure of a brittle material. The applied stress at the macroscopic scale is concentrated by the sharp geometry of the crack tip. The way the solid fails in response to the stress concentration is then determined by subtle lattice trapping and propagation instability effects which are controlled by atomic-scale chemical processes. Using up to date multiscale modelling strategies I will present several examples where details of the atomistic bond breaking processes lead to macroscopically observable differences in fracture behavior.

The second focus of this talk will be the simulation of friction and wear processes 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 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 the polishing of diamond proceeds.

Brief Biography:

Dr. Peter Gumbsch is a professor of Mechanics of Materials at the University of Karlsruhe (TH) and head of the Fraunhofer Institut for mechanics of materials IWM in Freiburg and Halle. His research activities focus on modelling and simulation of materials, in particular multiscale modelling approaches. His activities cover atomistic simulation, mesoscopic modelling as well as macroscopic materials descriptions. Central research topics are deformation and fracture processes as well as interface properties in metals and ceramics. He has recently started new activities in the area of tribology.

Dr. Gumbsch received the diploma degree in physics in 1988 and his PhD degree in 1991 from the University of Stuttgart. After extended visits at the Sandia National Laboratories in Livermore, postdoctoral work at the Imperial College, London and the University of Oxford he returned to the Max-Planck-Institut in Stuttgart as a group leader. In 2001 he took his current application-oriented position at Fraunhofer and the University of Karlsruhe. Dr. Peter Gumbsch is author of more than 120 refereed journal publications. Amongst other recognitions he was awarded the Otto Hahn Medal (1992), the Masing Memorial Award (1998), and the Gottfried Wilhelm Leibniz Prize (2007).