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Modeling contact, friction and wear: From atoms to the continuum

Lecture of

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Tribology is the science of mechanical processes at material surfaces, such as adhesion, friction or wear. Studying these is complicated because most surfaces are rough, interact with lubricants, water or air and because the interface between two materials is typically inaccessible to in-situ experimental techniques. In this talk, I give examples of how computer simulations at mesoscopic and atomic scales can help to elucidate the processes that take place at these “buried interfaces”. Mesoscopic simulations of elastic and plastic contact between rough surfaces allow a direct calculation of the area of intimate atomic contact and a prediction of macroscopic adhesive and frictional forces. Mechanical conditions within the contacting regions are typically extreme and give rise to severe plastic deformation. Plasticity leads to flattening of roughness but also to complex deformation patterns, such as vortices, underneath the surface. Molecular simulations of interfacial effects that occur in the region of intimate atomic contact during shear and of subsurface deformation shed light onto the microscopic mechanism governing near surface and subsurface deformation.