Computer Simulations of Soft Lithography: Crossover between Molecular and Macroscopic Properties

Andrey V. Dobrynin, Department of Physics, University of Connecticut

Adhesion phenomena play an important role in different areas of science and technology including tribology, colloidal science, materials science, biophysics and biochemistry. They are of paramount importance for nanofabrication and nanomolding, colloidal stabilization, drug delivery, interfacial friction and lubrication, cell mechanics and adhesion, and contact mechanics.

We have used molecular dynamics simulations and theoretical calculations to study peeling off of nanoparticles to understand static and dynamics of the nanoparticle adhesion. In our simulations we have calculated the potential of the mean force characterizing the strength of the nanoparticle interaction with the substrate as a function of the particle substrate separation. These simulations have shown that the detachment of the nanoparticle from substrate occurs through neck formation. The neck thickness decreases with increasing the nanoparticle shear modulus. Furthermore our simulations have shown that the critical detachment force and activation energy for nanoparticle detachment process are universal functions of the dimensionless parameter δ which is proportional to the ratio of the surface energy of a neck and the elastic energy of deformed nanoparticle.