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

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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 performed molecular dynamics simulations of pilling of nanoparticles to understand 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 established that the detachment time τ_R scales with the applied force as f^{-5}. This strong dependence is a result of the fine interplay between nanoparticle deformation and its adhesion to the substrate that control nanoparticle shape.