Abstract Submitted
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Dynamics of Nanoparticle Adhesion[1] J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut — We performed molecular dynamics simulations and theoretical analysis of nanoparticle pulling off from adhesive substrates. Our theoretical model of nanoparticle detachment is based on the Kramers solution of the stochastic barrier crossing in effective one dimensional potential well. The activation energy, ΔE, for nanoparticle detachment first decreases linearly with increasing the magnitude of the applied force, f, then it follows a power law $\Delta E \propto (f* - f)^{3/2}$as magnitude of the pulling force f approaches a critical detachment force value, $f*$. These two different regimes in activation energy dependence on magnitude of the applied force are confirmed by analyzing nanoparticle detachment in effective one dimensional potential obtained by Weighted Histogram Analysis Method. Simulations show that detachment of nanoparticle proceeds through neck formation such that magnitude of the activation energy is determined by balancing surface energy of the neck connecting particle to a substrate with elastic energy of nanoparticle deformation. In this regime the activation energy at zero applied force, ΔE_0, for nanoparticle with radius, R_p, shear modulus, G, surface energy, γ_p, and work of adhesion, W, is a universal function of the dimensionless parameter $\delta \propto \gamma_p W^{-2/3} (G R_p)^{-1/3}$. Simulation data are described by a scaling function $\Delta E_0 \propto \gamma_p^{5/2} R_p^{1/2} G^{-3/2} \delta^{-3.75}$. Molecular dynamics simulations of nanoparticle detachment show that the Kramers approach fails in the vicinity of the critical detachment force $f*$ where activation energy barrier becomes smaller than $k_B T$.

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