Abstract Submitted
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Contact Mechanics of Nanoparticles[1] J.-M.Y. CARRILLO, A.V. DOBRYNIN, University of Connecticut — We perform molecular dynamics simulations of the detachment of nanoparticles from a substrate. The critical detachment force, f^*, is obtained as a function of the nanoparticle radius, R_p, shear modulus, G, surface energy, γ_p, and work of adhesion, W. The magnitude of the detachment force is shown to increase from $\pi W R_p$ to $2.2\pi W R_p$ with increasing nanoparticle shear modulus and nanoparticle size. This variation of the detachment force is a manifestation of a neck formation upon nanoparticle detachment. Using scaling analysis, we show that the magnitude of the detachment force is controlled by the balance of the nanoparticle elastic energy, surface energy of the neck, and nanoparticle adhesion energy to a substrate. It is a function of the dimensionless parameter $\delta \propto \gamma_p (G R_p)^{-1/3} W^{-2/3}$which is proportional to the ratio of the surface energy of a neck and the elastic energy of deformed nanoparticle. In the case of small values of the parameter $\delta << 1$, the critical detachment force approaches a critical Johnson, Kendall and Roberts force, $f* \approx 1.5\pi W R_p$, as is usually the case for strongly crosslinked large nanoparticles. However, in the opposite limit, corresponding to soft small nanoparticles, for which $\delta >> 1$, the critical detachment force, f^*, scales as $f* \propto \gamma_p^{3/2} R_p^{1/2} G^{-1/2}$. Simulation data are described by a scaling function $f* \propto \gamma_p^{3/2} R_p^{1/2} G^{-1/2} \delta^{-1.89}$.

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