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Modeling Microcapsule-Substrate Interactions: Repairing Damages Surfaces and Separating Damaged Cells.

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We model two different scenarios that involve capturing the behavior of macromolecular assemblies. In the first study, we model the rolling motion of a fluid-driven, particle-filled microcapsule along a heterogeneous, adhesive substrate to determine how the release of the encapsulated nanoparticles can be harnessed to repair damage on the underlying surface. We integrate the lattice Boltzmann model for hydrodynamics and the lattice spring model for the micromechanics of elastic solids to capture the interactions between the elastic shell of the microcapsule and the surrounding fluids. A Brownian dynamics model is used to simulate the release of nanoparticles from the capsule and their diffusion into the surrounding solution. We focus on a substrate that contains a damaged region (e.g., a crack or eroded surface coating), which prevents the otherwise mobile capsule from rolling along the surface. We isolate conditions where nanoparticles released from the arrested capsule can repair the damage and thereby enable the capsules to again move along the substrate. Through these studies, we establish guidelines for designing particle-filled microcapsules that perform a "repair and go" function and thus, can be utilized to repair damage in microchannels and microfluidic devices. In the second study, we extend the above model of fluid-filled, elastic spheres rolling on substrates to three dimensions and thereby demonstrate a useful method for separating cells or microcapules by their compliance. In particular, we examine the fluid-driven motion of these capsules over a hard adhesive surface that contains soft stripes or a weakly adhesive surface that contains "sticky" stripes. As a result of their inherently different interactions with the heterogeneous substrate, particles with dissimilar stiffness are dispersed to distinct lateral locations on the surface. Since mechanically and chemically patterned surfaces can be readily fabricated through soft lithography and can easily be incorporated into microfluidic devices, our results point to a facile method for carrying out continuous "on the fly" separation processes.