255b Healing Surface Defects with Polymer Nanocomposites Containing Spheres and Rods

Kurt A. Smith, Sandeep Tyagi, and Anna Balazs

We use molecular dynamics (MD) simulations to investigate the benefits of applying a nanocomposite coating to substrates containing scratches and other defects. We consider a nanoparticle filled polymer film and show that the polymer melt induces a depletion attraction between nanoparticles and a flat surface. The nature of this force depends strongly on the particle shape, rodlike particles have a much stronger attraction than spherical particles. We quantify these interactions by measuring the effective potential between a particle and surface, as well as between two particles in the melt. We then consider the case of a surface notch, where the attraction is stronger due to the proximity of two surfaces. Here we show how tailoring the particle shape is a means of optimizing the tendency of particles to fill the notch. Morphologies obtained from the MD simulations are used as input to a lattice spring model which allows us to determine mechanical properties of the coated surfaces. The results show that the coating significantly reduces stress concentration at a notch. The application of such nanocomposite coatings could potentially yield defect-free surfaces that exhibit enhanced mechanical properties.