Molecular Simulation Study of Wetting at Rough Surfaces

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The manner in which a fluid wets a surface depends upon the energetic and structural characteristics of the substrate. The geometric roughness of the surface is known to play a significant role in this regard. This is evidenced by the successes and failures of things such as metal welded ceramics or water repellent fabrics. In this presentation we describe our recent computational work designed to better understand the influence of nanoscale (1-10 nm length scale) roughness on the wetting behavior of fluids. In this study we work with atomistically detailed substrates with measureable roughness. We use a Lennard-Jones fluid interacting with a substrate comprised of static particles. The particles are arranged in crystalline configurations and then etched to provide contours with nanoscopically-sized features. Grand canonical transition matrix Monte Carlo simulations are used to determine the surface free energy of a fluid in contact with a model surface. The free energy is then used to calculate spreading coefficients and contact angles. Our results indicate that both the amplitude and shape of substrate heterogeneities significantly alter the contact angle a fluid exhibits. We observe a switch from Wenzel-like to Cassie-like droplets as substrate features increase in amplitude or frequency. We also observe such a switch upon decreasing the strength of the substrate-fluid interaction. The results of our simulations are compared to the Wenzel and Cassie wetting models. In the case of Wenzel droplets, it appears that the relationship between contact angle and substrate roughness approaches that suggested by the Wenzel model as the length scale of the surface heterogeneities is increased.