Droplet dynamics on heterogeneous surfaces

Cem Servantie
Istanbul Technical University

We present molecular dynamics results on the dynamics of polymer droplets on smooth and patterned surfaces. The droplets are modeled as coarse-grained polymers in order to minimize the vapor pressure. The surface is made of two layers of fcc lattice, its hydrophilicity is controlled thanks to a modified Lennard-Jones potential. We use periodic boundary conditions in the direction transverse to the flow for computational efficiency. First we study the equilibrium and dynamic properties of droplets of varying sizes on different homogeneous surfaces. The equilibrium contact angles are evaluated. Next a bulk force is applied and the steady state velocity of the droplet as a function of the force is studied. We observe that for small enough accelerations –hence avoiding deformations of the droplets– the effective friction force due to the surface and the viscous dissipation is proportional to the velocity. We next focus on heterogeneous surfaces, now stripes of different hydrophilicity and widths are added to the surface. We show that the equilibrium contact angles on the heterogeneous surfaces are independent of the stripe widths if they are small enough, and correspond to the so-called Cassie-Baxter equation. We finally study the dynamics of the droplets on the striped surface, the simulations show that the droplets remain pinned on the surface if the bulk force is too small. Indeed, at equilibrium the droplet minimizes its free energy by maximizing its contact area with the hydrophilic stripes. This results in a net work required to depin the droplet, or in other words a static friction force. We show that the static friction force increases with the width of stripes. The results are explained by a simple model.