Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Kinetics of droplet wetting-mode transitions on grooved surfaces: Forward flux sampling AZAR SHAHRAZ, ALI BORHAN, KRISTEN FICHTHORN, Pennsylvania State University — Liquid droplets on rough surfaces typically exhibit either the Cassie wetting mode, in which the droplet resides on top of the roughness, or the Wenzel mode, in which the droplet penetrates into the roughness. For a fixed surface topology and droplet size, one of these modes is the global free-energy minimum. However, the other state is often metastable and long-lived due a free-energy barrier that hinders the transition between the two wetting states. Metastable wetting states have been observed experimentally and we also observe them in molecular dynamics (MD) simulations of a droplet on a grooved surface. Using forward flux sampling, we study the kinetics of the Cassie-Wenzel transition. The global-minimum wetting states that emerge from our nanoscale MD approach are consistent with those predicted by a macroscopic model for the free energy. We find that the free-energy barrier for this transition depends on the droplet size and surface topology. A committor analysis indicates that the transition-state ensemble consists of droplets that are on the verge of initiating/breaking contact with the substrate below the grooves.

Azar Shahraz
Pennsylvania State University

Date submitted: 26 Nov 2012 Electronic form version 1.4