Capillary Evaporation in Nonwettable Grooves

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We study liquid-gas phase transitions (i.e., capillary evaporation) in nanoscopic grooves of finite depth in the z- and width in the x-direction; the grooves are infinitely long in the y-direction. The interaction between a fluid (i.e., gas or liquid) molecule with the groove walls is purely repulsive, that is the grooves are not wet by the fluid material. We employ Monte Carlo simulations in the grand canonical ensemble to investigate the impact of groove geometry on capillary evaporation. The fluid inside the grooves is coupled to a reservoir of matter such that the grooves can exchange matter with the remainder of the system through purely diffusive processes. We focus on the thermodynamic conditions under which the fluid outside the groove already underwent a phase transition from gas to liquid, whereas the fluid inside the grooves turns out to still be gaseous in nature. In some simulations we also model the liquid outside the grooves by means of an effective potential depending on the thermodynamic state of the liquid. This permits us to speed up the simulations significantly so that the groove geometry can be varied over a wide range of sizes. Our results indicate that for small grooves capillary evaporation gives way to a continuous filling process. Moreover, we compare results obtained for finite-size grooves with those obtained for corresponding slit-pores which are infinitely large in two dimensions rather than one. This comparison permits insight into finite-size effects on drying at nonplanar solid surfaces.