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Evaporation of Sessile Droplets on Nanopillared Surfaces

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Droplet evaporation is not only a fundamental phenomenon in nature, but also very important in biomedical and modern engineering applications. [1, 2] During the evaporation of a sessile droplet, the dynamics of the contact line is also involved. [3] One of the major issues is the mechanism of the pinning and depinning of the contact line (CL), which is essential in understanding the evaporation mode transitions. [4]

In this work, pinning and depinning mechanisms of the contact line during evaporation of the sessile droplets on solid surfaces with nanopillars were investigated using molecular dynamics (MD) simulations. [5] Evaporation of the sessile nano-droplet takes two steps in the MD simulations. First, to judge whether a water molecule is on the surface or in the bulk, we calculated the centro-symmetry parameter (CSP). Then, a certain number of water molecules on the surface were picked randomly and deleted at regular intervals. This approach aimed to imitate the transition of molecules from liquid to gas phase.

To investigate the pinning and depinning of the contact line during evaporation, we compared evaporation behavior on nanopillared substrates with different morphology. There exist three evaporation modes for sessile droplets: the constant contact radius (CCR) mode, the constant contact angle (CCA) mode and the mixed mode which usually takes place at the end of evaporation. The transition of evaporation mode from CCR to CCA is associated with the stick-slip dynamics of the contact line. During the evaporation, the out-of-balance surface tension promoted the receding of the contact line, while the pinning force acts to obstruct the motion. For the evaporation of sessile droplets on nanopillared surfaces, we should consider the energy barrier for the contact line to jump from one nanopillar to another.

Our MD results have shown that the surface wettability as well as the characteristic width of the nanopillar has a significant influence on the behavior of the contact line motion. For the solid surfaces with hydrophilic nanopillars, the contact line is pinned on the surface during the evaporation and exhibits the CCR mode. For the solid surfaces with hydrophobic nanopillars, the evaporation of the nanodroplet switches between the CCA mode and the CCR mode, which indicates that the contact line motion show the stick-slip behaviour. These findings enhance our understanding on the liquid-solid interactions at the atomic scale. Moreover, our results indicated that by choosing the surface property and morphology, the evaporation behaviour can be actively controlled for specific applications such as nanoassembly as well as DNA stretching. [6, 7]

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