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Phase Diagram of Impacting Nanodroplets on Mesh Surfaces

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ABSTRACT

Controlling dynamics of impacting droplets on meshes is significantly important, which attracted a lot of attention because of its great potential applications in liquid separation, self-cleaning, and water harvesting [1-3], yet the underlying physical mechanisms are not entirely revealed. Here, the impact dynamics of a nanodroplet on mesh surfaces with different wettability are studied through molecular dynamics (MD) simulations. Due to scale effects between the nano and macroscale, the impacting nanodroplets exhibit some unique dynamic characteristics [4-7]. On a superhydrophobic mesh surface, when varying the impact conditions of nanodroplets, different outcomes can occur: (i) at a small impact *We*, the nanodroplet is entirely captured by the mesh; (ii) increase *We*, part of droplets penetrate through the mesh without breaking up; (iii) above a threshold *We*, some satellite droplets are ejected below the surface. Based on the impacting outcomes, a phase diagram is established in the parameter space of *We* against the surface structure dimension. The effect of wettability on penetration is validated in a wide range of static contact angles from hydrophilic to superhydrophobic surfaces. Finally, in the phase diagram, the boundaries of different outcomes are analyzed. It is found that the existing models are not suitable here due to the enhanced viscous effect of impacting nanodroplets[8]. A theoretical model is developed to propose critical conditions for the penetration with break out, which agree well with the boundary in the phase diagram. The findings in this work provide rational design principles for regulating the controllable penetration on mesh surfaces in a wide range of applications.

KEYWORDS

Nanodroplet impact; mesh surface; wettability; molecular dynamics

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