Line tension and wettability of nanodrops on curved surfaces

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Abstract

We have studied the formation of nanodrops on curved surfaces (both convex and concave) by means of molecular dynamics simulations, where the particles interact via a Lennard-Jones potential. We found that the contact angle is not affected by the curvature of the substrate, in agreement with previous experimental findings. This means that the change in curvature of the drop in response to the change in curvature of the substrate can be predicted from simple geometrical considerations, under the assumption that the drop fits a spherical cap, and that the volume remains the same. We found that this prediction was in perfect agreement with the simulation results, for both convex and concave substrates. We have calculated the line tension by fitting the data for the contact angle for different size drops to modified Young’s equation. The magnitude of line tension calculated from our simulations is in the range of calculated from theoretical predictions. We have found that the line tension depends on the nature of the surface curvature. Magnitude of the line tension is much more in case of concave surfaces when compared with convex surfaces and maximum in case of zero curvature.

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