Contact-line fluctuations and dynamic wetting

Experiment shows that advancing contact angles increase with contact- line velocity, while receding contact angles decrease. Although there are several theories to explain why [1], they all involve parameters that must be obtained by fitting experimental data. As a consequence, it remains impossible to predict from first principles how a liquid drop will evolve with time or how the dynamic contact angle will change with velocity. However, given the strong relevance of wetting to nanotechnology, it is essential to have a sound theoretical understanding of the process at the same scale.

From a macroscopic perspective, a liquid drop at equilibrium may appear to be at rest. But at the molecular level, because of thermal fluctuations, the picture is far from static. This is true not only for the bulk liquid, but also the liquid–solid and liquid–vapor interfaces. It will, therefore, also be true for the three-phase contact. In consequence, the contact line will constantly fluctuate about some mean configuration and position [2]. In this work [3], we show that these fluctuations are crucial to our understanding of dynamic wetting at the nanoscale.

We use large-scale molecular dynamics simulations to model a liquid bridge between two molecularly smooth solid surfaces and study the positional fluctuations of the contact lines so formed as a function of the solid-liquid interaction. Our study shows that these thermal fluctuations may be modeled as an overdamped one-dimensional Langevin oscillator and they can be used to determine key parameters that control dynamic wetting. We then compare these coefficients with those obtained by measuring the dynamic contact angle as a function of contact- line speed in independent simulations and applying the molecular-kinetic theory of dynamic wetting. We find excellent agreement between the two. As well as providing further evidence for the underlying validity of the molecular-kinetic model, our results suggest that it should be possible to predict the dynamics of wetting by experimentally measuring the fluctuations of the contact line of a capillary system at equilibrium. This would circumvent the need to measure the microscopic dynamic contact angle directly.

References

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