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Stick-Slip Motion of Moving Contact Line on Chemically Patterned Surfaces

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Abstract. Based on our continuum hydrodynamic model for immiscible two-phase flows at solid surfaces, the stick-slip motion has been predicted for moving contact line at chemically patterned surfaces [Wang et al., J. Fluid Mech., 605 (2008), pp. 59-78]. In this paper we show that the continuum predictions can be quantitatively verified by molecular dynamics (MD) simulations. Our MD simulations are carried out for two immiscible Lennard-Jones fluids confined by two planar solid walls in Poiseuille flow geometry. In particular, one solid surface is chemically patterned with alternating stripes. For comparison, the continuum model is numerically solved using material parameters directly measured in MD simulations. From oscillatory fluid-fluid interface to intermittent stick-slip motion of moving contact line, we have quantitative agreement between the continuum and MD results. This agreement is attributed to the accurate description down to molecular scale by the generalized Navier boundary condition in our continuum model. Numerical results are also presented for the relaxational dynamics of fluid-fluid interface, in agreement with a theoretical analysis based on the Onsager principle of minimum energy dissipation.

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Key words: Moving contact line, slip boundary condition, patterned surface.

1 Introduction

The contact line denotes the intersection of the fluid-fluid interface with the solid wall in immiscible two-phase flows. When one fluid displaces the other, the contact line moves

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along the wall. As a classical problem in continuum hydrodynamics, it has been known for decades that the moving contact line is incompatible with the no-slip boundary condition [1] — the latter leads to a non-integrable singularity in viscous dissipation [2–4]. In particular, molecular dynamics (MD) simulations have shown that near-complete slip indeed occurs at the moving contact line [5, 6]. Numerous models were proposed to address this problem, but none was able to give a quantitative account of the MD slip velocity in the molecular-scale vicinity of the contact line [7–15].

Through analysis of extensive MD data, it was discovered that the slip velocity measured in nanoscale MD simulations satisfies the generalized Navier boundary condition (GNBC) [16]. The GNBC states that the relative slip velocity between the fluid and the solid wall is proportional to the total tangential stress — the sum of the viscous stress and the uncompensated Young stress; the latter arises from the deviation of the fluid-fluid interface from its static configuration. By the use of the Cahn-Hilliard (CH) hydrodynamic formulation for two-phase flows [13, 14, 17], the implementation of the GNBC leads to continuum solutions in quantitative agreement with MD simulation results [16, 18, 19]. Recently, it has been shown [20, 21] that the GNBC can be derived in a variational approach from the Onsager principle of minimum energy dissipation [22,23].

Recently, structured surfaces exhibiting lateral patterns of varying wettability have become technically available. The morphologies of liquid on patterned surfaces with hydrophilic and hydrophobic regions have been investigated experimentally and theoretically [24,25]. While the statics of wetting on patterned surfaces already leads to a large variety of morphologies, the dynamics of wetting on these surfaces is even more complicated. Cubaud and Fermigier carried out an experimental investigation on the advancing contact lines of large drops spreading on chemically patterned surfaces [26]. In a numerical study for an immiscible two-phase fluid driven to flow past chemically patterned surfaces in a microchannel, Kuksenok *et al.* showed that the fluid exhibits morphological instabilities giving rise to the formation of monodisperse droplets of one phase in the other phase [27]. Through both numerical simulations and experiments, Kusumaatmaja *et al.* explored the behavior of liquid drops moving past a surface patterned with hydrophobic and hydrophilic stripes [28].

We would like to point out that in all the previous studies based on diffuse-interface modeling [12–15, 27, 28], the no-slip boundary condition is kept and the non-integrable stress singularity is removed by introducing diffusive transport through the fluid-fluid interface. By combining the GNBC with the diffuse-interface formulation, our continuum model allows the coexistence of slip and diffusion, with their competition determined by the relative magnitudes of relevant parameters [20]. For the systems simulated in our MD study, it is the slip that dominates. A recent study by Ren and E [29], which focused on a sharp interface model, also demonstrated that the stress singularity is regularized by the existence of a slip region and the Young stress is dominant in the contact line region. We have applied our model to further investigate the role of slip for contact line motion at surfaces patterned with stripes of varying contact angle [30]. We found that as the fluid-fluid interface is displaced along the patterned surface, its shape is periodically