Electronic Supplementary Material (ESI) for Soft Matter

Supporting material: simulation details

We model the system as a diffuse-interface, two-phase fluid in contact with a solid substrate. The thermodynamic state of the fluid is described by an order parameter $\rho(\boldsymbol{r})$, corresponding to the density of the fluid at each point $\boldsymbol{r}$. The equilibrium properties are modelled by a Landau free energy functional over the spatial domain of the fluid $\mathcal{D}$, and its boundary with solid surfaces $\partial\mathcal{D}$, as [1]

$$\Psi = \iiint_{\mathcal{D}} (p_c\left\{\nu^4 - 2\beta\tau_W\left(1-\nu^2\right)-1\right\} - \mu_b\rho + \frac{1}{2}\kappa\left|\nabla\rho\right|^2)dV - \iint_{\partial\mathcal{D}} \mu_s\rho dS. \quad (1)$$

The first term in the integrand of (4) is the bulk free energy density, where $\nu = (\rho-\rho_c)/\rho_c$ and ρ_c, p_c, and $\beta\tau_W$ are constants. It allows two equilibrium bulk phases, liquid and gas, with $\nu = \pm\sqrt{\beta\tau_W}$. The second term is a Lagrange multiplier constraining the total mass of the fluid. The third term is a free energy cost associated with density gradients. This allows for a finite width, or diffuse, interface to arise between the bulk phases, with surface tension $\gamma = \frac{4}{3}\rho_c\sqrt{2\kappa p_c(\beta\tau_W)^3}$ and width $\chi = \frac{1}{2}\rho_c\sqrt{\kappa(\beta\tau_W p_c)^{-1}}$. The boundary integral takes the form proposed by Cahn.[2] Minimizing the free energy leads to a Neumann condition on the density

$$\partial_\perp\rho = -\frac{\mu_s}{\kappa}. \quad (2)$$

The wetting potential μ_s is related to the Young angle δ of the substrate by [1]

$$\mu_s = 2\beta\tau_W\sqrt{2p_c\kappa}\ \mathrm{sign}(\frac{\pi}{2}-\delta)\sqrt{\cos\frac{\alpha}{3}(1-\cos\frac{\alpha}{3})} \quad \text{with} \quad \alpha = \arccos(\sin^2\delta). \quad (3)$$

The hydrodynamics of the fluid is described by the continuity and the Navier-Stokes equations

$$\partial_t\rho + \partial_\alpha\left(\rho u_\alpha\right) = 0 \quad (4)$$

$$\partial_t\left(\rho u_\alpha\right) + \partial_\beta\left(\rho u_\alpha u_\beta\right) = -\partial_\beta P_{\alpha\beta} + \partial_\beta\left(\rho\eta\left(\partial_\beta u_\alpha + \partial_\alpha u_\beta\right) + \rho\lambda\delta_{\alpha\beta}\partial_\gamma u_\gamma\right), \quad (5)$$

where u is the local velocity, P is the pressure tensor derived from the free energy functional (1) as

$$P_{\alpha\beta} = \left(p_c\left(\nu+1\right)^2\left(3\nu^2 - 2\nu + 1 - \beta\tau_W\right) - \frac{1}{2}\kappa\partial_\gamma\rho\partial_\gamma\rho - \kappa\rho\partial_{\gamma\gamma}\rho\right)\delta_{\alpha\beta} + \kappa\partial_\alpha\rho\partial_\beta\rho, \quad (6)$$

with $\eta = \frac{\Delta t}{3}(\tau - \frac{1}{2})$ and $\lambda = \eta(1 - 12p_c\rho_c^{-2}\rho\left(3\nu^2 - \beta\tau_W\right))$ are the shear and bulk kinematic viscosities respectively. A free energy lattice Boltzmann algorithm is used to numerically solve equations 7 and 8.[3–5] At the substrate we impose the boundary condition (5),[1,6] and a condition of no-slip.[7–9] We choose $\kappa = 0.01$, $p_c = 0.125$, $\rho_c = 3.5$, $\tau_W = 0.3$ and $\beta = 1.0$, giving an interfacial thickness $\chi = 0.9$, surface tension $\gamma = 0.029$ and a density ratio of 3.42. The viscosity ratio is $\eta_L/\eta_G = 7.5$.

We concentrate our attention on substrates patterned with hexagonal arrays of posts with equilateral triangles as cross-sections. The posts have height $h = 20\,l.u.$ (lattice units or cells), side length $b = 20\,l.u.$, and centre-to-centre separation $d = 40\,l.u.$. The posts and the base substrate have the same Young angle δ.

References

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