Crossover of Dynamic Wetting Regimes: a Molecular Dynamics Study

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The dynamic spreading regime in the complete wetting case of advancing contact line motion features a transition when the contact line speed approaches a critical value from above and an advancing precursor film starts to appear. In the study, which is a sequel of our previous investigation of the dynamic contact angle mechanism, **ACS Nano**, (2016), **10**: 6045-6053, we analyze a crossover between the two dynamic wetting states, with and without the precursor film, using molecular dynamics simulations. We investigate, from the first microscopic principles, characteristic features of the onset of the precursor film and its relationship with the dynamic contact angle. Remarkably, though could be expected, we observed that even when the precursor film was well developed, the dynamic contact angle θ_c (as is illustrated) was still defined by the whole area covered by the precursor film.

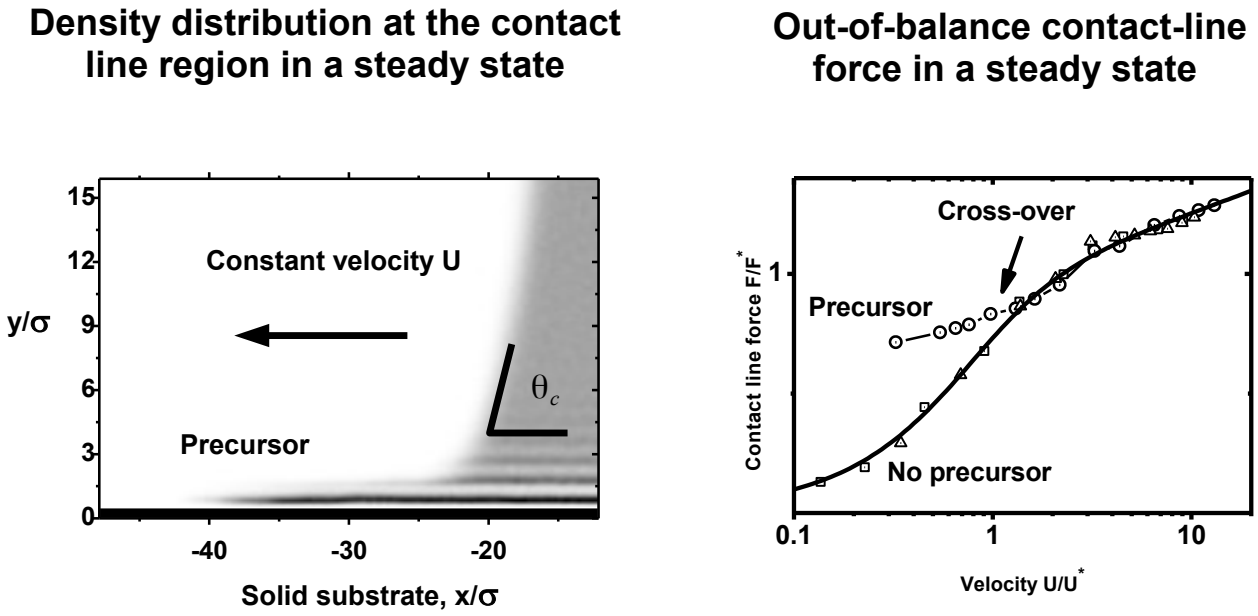

Figure 1: Illustration of the onset of the **precursor** film in advancing contact line motion - **MDS**. **Density distribution** (liquid is shown in dark colour) in complete wetting case and the out-of-balance **contact line force** $F/F^\star = \gamma_{GS} - \gamma_{LS} - \gamma\cos\theta_c$ as a function of normalized velocity $U/U^\star$ in complete wetting (static angle $\theta_S = 0$, precursor present) and incomplete wetting (static angle $\theta_S > 0$, no precursor) cases.

Keywords: *wetting, nano-scale, contact line, macroscopic boundary conditions, molecular dynamics simulations.*