POSTER

Density Distributions and Diffusivities - Implications for Slip at Solid-Liquid Interfaces

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Experimental evidence is accumulating for slip at solid-liquid interfaces from a wide range of sources. Slip has implications in areas such as polymer processing and for flow in microchannels. Slip is often introduced to partially overcome the problem of describing how a dynamic wetting line moves across a solid surface and is therefore relevant to current models of coating.

It is widely believed that parameters such as the slip length will depend on the strength of solid-liquid interactions (i.e. the wettability of the substrate), and indeed such effects have been reported. Nevertheless, there is no consensus about the magnitude of this effect, let alone the detailed mechanism. A molecular model for slip was first proposed by Tolstoi in 1952, but although it seems to predict experimentally observed trends, it has never really been tested. Here we report the use of large-scale molecular dynamics simulations to study the mobility of molecules near the wall as a function of solid-liquid interactions and to simultaneously investigate the dynamics of wetting in these systems. The results of these combined simulations are being used to probe the utility of the Tolstoi model, to investigate some alternative hypotheses, and show a tentative link with the dynamics of wetting.