YOUNG'S EQUATION AND NANOTUBES

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Keywords: Young's equation, nanotube, molecular dynamics, capillary force

Recently [1], the use of Young's equation which predicts that $\gamma_{SV} = \gamma_{SL} + \gamma_{LV}\cos\theta^0$ where γ_{SV}, γ_{SL}, γ_{LV} are respectively the solid/vapor, solid/liquid, and liquid/vapor surface tensions and θ^0 the static contact angle measured from the solid, inside the liquid, at the contact line, has been justified at the nanoscale via the analysis of the distribution of forces exerted by a Lennard-Jones liquid along a nanofiber modelled by large-scale molecular dynamics (MD). This current study extends this work by investigating the wettability of nanotubes, i.e. nanofibers opened at both ends. This is a necessary step to fully validate the use of Atomic Force Microscope experiments routinely employed to characterize the wettability of nanoparticles and especially carbon nanotubes [2].

In our MD simulations, all potentials between atoms, solid as well as liquid, are described by modified pair-wise Lennard-Jones 12-6 interactions, where various parameters are adjusted to enhance or inhibit both the spreading of the liquid around the tube and its filling (Figure 1) [3]. The associated static contact angles around the tube, the forces induced by the liquid at the bottom, at the contact line, and at the top of the tube were then calculated independently. Figure 2 compares the force distributions for a nanofiber and a nanotube at equilibrium. For a nanofiber and a non-wettable nanotube (θ^0>90°), forces per unit length are measured at its bottom (γ_{LV}) and at the contact line ($-\gamma_{LV}(1+\cos\theta^0)$) leading to a net force ($-\gamma_{LV}\cos\theta^0$) predicted by Young's equation [1]. When the liquid imbibes the tube (θ^0<90°), an additional force is measured at its top, pulling on it. In addition, an increase of the force exerted at its bottom, pushing in the opposite direction, is observed. The force at the contact line remains identical to the one measures for a nanofiber. If the distributions of forces are different for a nanofiber and a wettable nanotube, the net force remains however the one predicted by Young's equation. Again, it is a strong evidence that it is valid down to the molecular scale.

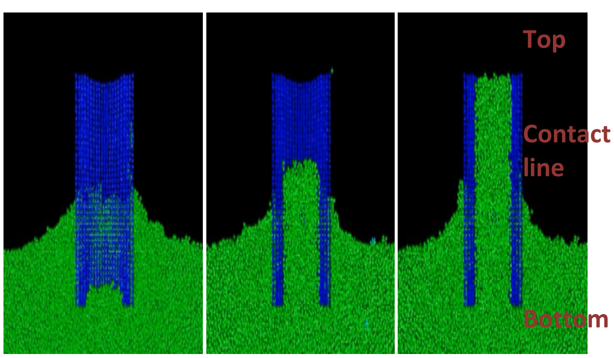

Figure 1: Filling of a 8 nm diameter nanotube tube by a Lennard-Jones liquid (from left to right). The liquid exerts forces at the top and at the bottom of the tube as well as around it at the contact line.

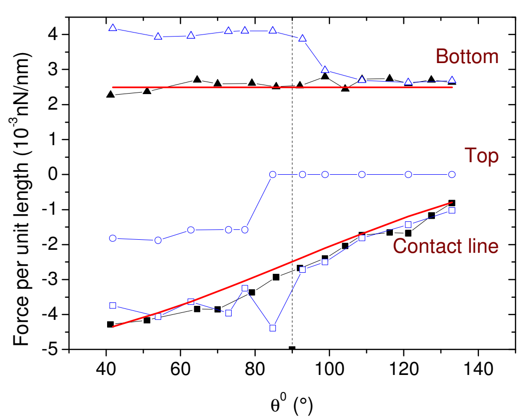

Figure 2: Force distribution along a nanofiber (Black symbol) and a nanotube (Blue symbol) at equilibrium plotted as a function of the equilibrium contact angle. The full red lines represent γ_{LV} and $-\gamma_{LV}(1+\cos\theta^0)$.

1. D. Seveno, T. D. Blake, J. De Coninck, Phys. Rev. Lett. 111, 096101, 2013
2. A.H. Barber, S.R. Cohen, H.D. Wagner, Phys. Rev. B 71, 115443, 2005
3. G. Martic, F. Gentner, D. Seveno, D. Coulon, J. De Coninck, Langmuir 18, 7971, 2002