Forces within Three Phase Contact Zone: a mechanical interpretation of Young's equation at the nanoscale

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Abstract

Thomas Young first described the value of the equilibrium contact angle of a liquid on a solid in 1805, known as Young's equation. Over the past 200 years, efforts have been made to interpret this equation. However, the mechanical interpretation still remains unclear at the nanoscale. Using molecular dynamics simulations, we model a liquid droplet on a flat solid substrate and investigate the mechanical equilibrium of the system at the three phase contact zone (TPZ). We first confirm that the equilibrium of the liquid droplet is only controlled by the interactions at the contact line. Both normal and tangential forces exerted by the liquid on the solid are described in quantitative terms, which is in agreement with the Young's equation when contact angle is relatively large. However, when contact angle is small, the liquid meniscus becomes thin and the surface tension of the liquid decreases, resulting in the decrease of forces on the solid. Furthermore, by modeling liquid-solid systems with LJ 9-3 interaction, we find that surface tension of the liquid near the liquid-solid interface is different from that near the liquid-vapor interface and is affected by the strength of liquid-solid interaction. Based on these characterizations, we proposed a novel theoretical description of the mechanical equilibrium at the TPZ and the theoretically predicted tangential force shows good agreement with that measured in the TPZ. Our findings give a detailed mechanical interpretation of Young's equation at the nanoscale and may provide guidance when applying Young's equation in nanotechnology.

Keywords: **Wetting, Young's equation, Contact line, Liquid-solid interface, Molecular dynamics simulation**