A study of water droplet between an AFM tip and a substrate using dissipative particle dynamics

SOUVIK PAL, CHUANJIN LAN, University of California, Merced, ZHEN LI, Brown University, E. DANIEL HIRLEMAN, YANBAO MA, University of California, Merced — Formation of a water droplet between a sharp AFM tip and a substrate due to capillary condensation affects the tip-substrate interaction. As a consequence, AFM measurements lose precision and often produce incorrect sample topology. Understanding the physics of liquid bridges is also important in the field of Dip-pen nanolithography (DPN). Significant research is being carried out to understand the mechanics of the formation of the liquid bridge and its dependence of surface properties, ambient conditions etc. The in-between length scale, i.e., mesoscale (∼100 nm) associated with this phenomenon presents a steep challenge for experimental measurements. In addition, molecular dynamics (MD) can be computationally prohibitive to model the entire system, especially over microseconds to seconds. Theoretical analysis using Young Laplace equation has so far provided some qualitative insights only. We study this system using Dissipative Particle Dynamics (DPD) which is a simulation technique suitable for describing mesoscopic hydrodynamic behavior of fluids. In this work, we carry out simulations to improve understanding of the process of formation of the meniscus, the mechanics of manipulation and control of its shape, and better estimation of capillary forces. The knowledge gained through our study will help in correcting the AFM measurements affected by capillary condensation. Moreover, it will improve understanding of more accurate droplet manipulation in DPN.