Wetting Transition of a nano drop on switchable hydrophobic-hydrophilic surfaces

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Introduction

- The wetting properties of materials are largely dictated by the contact angle of the liquid which is in contact with the solid surface and the solid-liquid surface tension properties.
- There are plenty of industrial, biological and manufacturing applications which are primarily based on phenomena of rapid wetting.[1] On the other hand, there are applications which requires poor wetting.[2]
- The scientific community is mostly focused towards the understanding of wetting behavior and designing materials or surfaces of desired engineering applications.
- Due to lack of experimental methods for measuring the contact angle and various experimental challenges related to small length scale, molecular simulation is one of the viable option in predicting the preliminary insights of molecular level vision of liquids and their interfacial properties.
- it is obvious that the surface properties can modulate the wettability of the drop. The nature of the surface can be modified by external stimuli. It would be a great advantage where the surface properties can be controlled, resulting in a controlled wetting and dewetting characteristic of the nano droplet.
- In this work, a wetting and dewetting characteristics of a nano water droplet in contact with a conductive tip and placed on a perpendicular insulator surface, which is contact with a planar electrode layer, has been studied using atomistic molecular simulation.

Methodology

- The present simulation system consists of a water nano drop in contact with a conductive tip and wetting a perpendicular planar electrode covered by an insulator layer as shown in Fig. 1.
- At the bottom of the insulator layer two planar platinum electrodes are placed. The Pt layers are 98 angstrom cubic simulation volume obtained by cutting a face centered cubic platinum crystal with lattice parameter 3.9 angstrom along the (1 1 1) crystallographic plane.
- Below the insulator layer two platinum layers are placed. Basically this simulation system represents a typical setup of electrowetting-on-dielectric (EWOD) experiment.
- In this way the platinum layer consists of 2500 atoms, while the insulator layer counts 1250 atoms. The counter electrode is a cylindrical platinum rod attached with a hemispherical tip which is placed
perpendicular to the planar electrode. The tip consists of 546 Pt atoms.
- At the beginning of the simulation the tip is inserted inside 2000 water molecules nano drop. The molecules overlapping the Pt atoms has been removed and the final number of water molecules inside the drop is 1900. Now a molecular dynamics is performed for the whole system by fixing the surface atoms.

Figure # 1

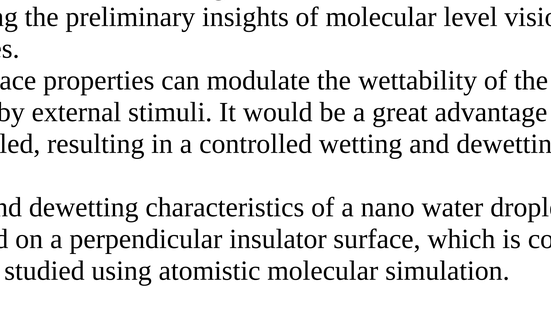
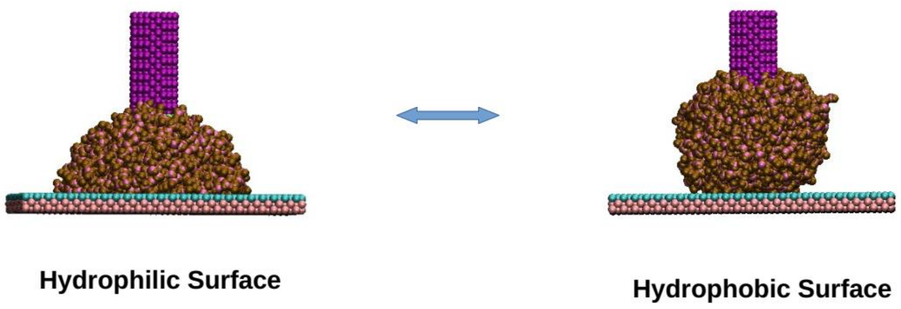


Figure # 2



Results

- Figure 2 shows the effect of surface on the drop.
- Figure 3 shows the variation of the height of the center of mass of the drop with time.

Figure # 3

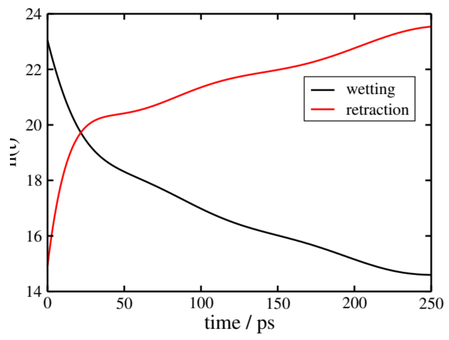
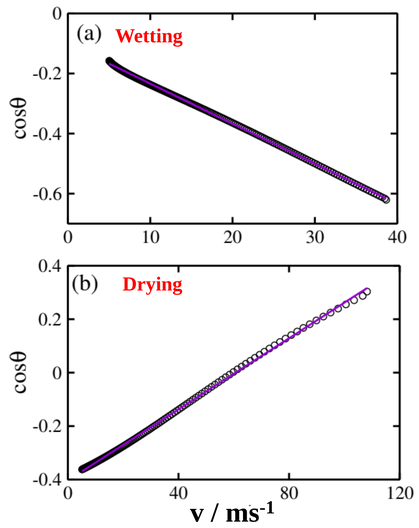


Figure # 4



Molecular Kinetic Theory (MKT)[3]:

- It concerns thermally activated displacements of liquid molecules at the three phase contact line. Individual molecular jumps occur with a characteristic frequency k_0 and length λ. The relation between the dynamic contact angle and the perimeter velocity (v) is given by

$$v = 2k_0\lambda \sinh\left[\frac{\gamma_{lv}\lambda^2}{2k_BT}(\cos\theta_0 - \cos\theta)\right]$$

- k_B is the Boltzmann constant and T temperature. For small arguments of sinh,

$$v = \frac{\gamma_{lv}(\cos\theta_0 - \cos\theta)}{\zeta} \qquad \zeta = \frac{k_BT}{k_0\lambda^3}$$

Figure # 5

Figure # 6

Conclusions

- The molecular insight of the wetting of nano drop is presented using Molecular dynamics simulation.
- The study demonstrates a reversible switching of the droplet's contact angle regarding the switchablity of the surface properties.
- The analysis of the droplet relaxation rates shows that the retraction is considerably faster than the spreading.
- The phenomena is explained liquid/solid friction under the propagating droplet perimeter as formulated in the molecular kinetic theory.[4]
- The study also invites applications in the dynamic control of permeation in hydrophobic nanopores for nanofluidic devices.

Bibliography

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