Molecular simulation of fluid-solid interfaces at nanoscale

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Abstract :

The equilibrium states of vapor and liquid coexistent phases in contact with a solid surface are studied at the nanoscale by molecular dynamics simulations for a temperature close to the fluid triple point. The characteristics of the solid-fluid interfaces are determined when the interaction strength between the fluid and the solid varies in order to go from a situation of complete drying to that of complete wetting. From the vapor-liquid density profiles of liquid drops lying on the substrate surface or menisci of liquid films confined in slit pores, the contact angles made by the vapor-liquid interface with the solid are computed. The angle values are similar for the drops and the films. They are also in good qualitative agreement with the estimates obtained through the Young's relation from the surface tensions associated with the vapor-solid, liquid-solid, and vapor-liquid interfaces. However, at this scale, the uncertainties inherent to the angle computation and, to a lesser extent, to size effects seem to preclude that the quantitative agreement between the angle estimates obtained from the interface geometry and calculated from the Young's relation can be better than few degrees.

Keywords : molecular dynamics method, solid-liquid transformations, surface tension.

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