IMPACT OF NANODROPS ON SMOOTH SURFACE WITH VARIOUS WETTABILITIES

B.Braeckeveldt[1], M.Marengo[2], J.C.Fernandez Toledano[1], J.De Coninck[1]

[1]UMONS, Mons, Belgium; [2]University of Brighton, Brighton, U.K.

joel.deconinck@umons.ac.be

Interaction of nanodroplet with surfaces is a fascinating novel subject with potential major impact for nanomedicine, 3D nanoprinting, nanoscale liquid impingement, phase-change cooling using nanosprays and for special material microdeposition processes. The impact of nanometric drops on smooth solid surfaces is studied using molecular dynamics simulations. Using LAMMPS software, we study in details the impact of slice of drops on substrates. This allows us to model considerably large drops in a reasonable simulation time. We have first validated this approach by studying the dynamics of spontaneous spreading for the corresponding sliced droplet. We prove that this technique allows to recover exactly previous simulated results obtained for truly three dimensional nanodroplets modelled under the same conditions [1]. We then generalize this study by considering an initial impact velocity. Nanodrops impacting at low velocity bounce from non-wetting surfaces but stick and subsequently spread on wetting surfaces. Droplet impact can also be studied in the case of a wetted substrate. In this case, an application is to use the energy of impact to break the liquid film and initiate dewetting. High impact velocities onto a wetted surface produce a crown splash like usually observed for macroscopic drops. Impact velocity, liquid-solid affinity and film thickness are the parameters which affect dewetting [2]. Increasing the velocity of the droplet will help to dewet, while increasing the liquid-solid affinity will lead to more resistant film. Our preliminary simulations confirm these results. Even if drop spreading can be analysed in terms of Weber and Reynolds as for millimetric droplets, a modification of the standard map of the impact regimes is necessary to take into account the adhesion forces between the liquid and the solid surface at the nanometric scale. Our molecular dynamics simulations provide a detailed look in the mechanisms that connect the drop impact with splash and dewetting phenomena. A precise description of this phenomena at the nanoscale could provide an accurate estimation of the maximal impact velocity to obtain a smooth and homogenous coverage of the surfaces without dry spots. Therefore it could improve the design of interesting techniques as nanoprinting. Results are also encouraging and stimulating to study heat transfer at the nanoscale during dewetting, for example to characterize the start of the Leidenfrost process.

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