Impact of nanodrops on smooth surfaces with various wettabilities: splash phenomena and film dewetting

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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 nanometer sized 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 to consider in a reasonable amount of time systems which can reach significantly larger sizes along the x-z directions. We have first validated this approach by studying the dynamics of spontaneous wetting for the corresponding sliced droplet. We prove that this technique allows to recover exactly previous results obtained for truly three dimensional nanodroplets in the same conditions. We then generalize this study by considering an impact speed. Nanodrops impacting at low velocity bounce from non-wetting surfaces but stick and subsequently spread on wetting surfaces. Higher velocity impacts onto a wetted surface produce a crown splash like it is usually observed for larger drops. Impact velocity, liquid-solid coupling and film thickness are the parameters which affect dewetting. Increasing the velocity of the droplet will help to dewet while increasing the coupling will lead to more resistant film. Results showed that the dewetting speed depends on the thickness of the film and the coupling. Even if the 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 atomic solid surface. Our results show the ability of molecular dynamics to provide a detailed look on how impact can induce a splash and a dewetting phenomenon. This may help the design of nanoprinters, since it is giving an estimation of the maximum impact velocities in order to obtain a smooth and homogenous coverage of the surfaces without dry spots. Results are also encouraging and stimulating to use these techniques to study heat transfer at the nanoscale during dewetting.