Chapter 7
Conclusions and Prospects

Abstract In this chapter, we provide the general conclusions and the contributions of this book. The prospects in dynamic wetting by nanofluids are also provided in this chapter.

7.1 Conclusions

Due to their special flow and thermal properties, nanofluids were widely used in heat transfer enhancement and drag reduction devices, as well as in the drug delivery and micro/biofluid systems, in which the dynamic wetting by nanofluids plays significant roles. The mechanism of dynamic wetting by nanofluids is still unclear due to limitations of nanoscale experimental techniques and fundamental theories. Studies of the dynamic wetting by nanofluids face great challenges since the wetting behavior crosses several length and timescales. This book analyzes the effects of the bulk and local dissipation in the nanofluids due to the transport and self-assembly of nanoparticles on the macroscopic dynamic wetting behavior using macroscopic experiments and multiscale simulation methods. The results describe both the macroscopic and microscopic mechanisms and tunable methods to control nanofluid dynamic wetting. The main conclusions are as follows:

1. The time-dependent wetting radius and contact angle for various dilute nanofluid droplets were measured by the droplet spreading method. The effects of the nanoparticle material, loading and diameter, the base fluid, and the substrate material were examined. The results show that the adding of nanoparticles inhibits the dynamic wetting of nanofluids as compared with base fluids. The reduced spreading rate can be attributed to the increase in either surface tension or viscosity due to adding nanoparticles into the base fluid. It is interesting that once the effects of the surface tension and viscosity are both eliminated using the non-dimensional analysis, the wetting radius versus spreading time curves for all the nanofluid droplets overlap each other. In addition, the spreading exponent fitted from the nanofluid dynamic wetting data is found to be very close to 0.1,

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which meets the prediction of the classical hydrodynamic model derived from the bulk viscous dissipation approach. Thus, the present results prove that the spreading of the dilute nanofluid droplets is dominated by the bulk dissipation rather than by the local dissipation at the moving contact line.

2. The dynamic spreading of water nanodroplets containing non-surfactant nanoparticles and the effects of structural disjoining pressure are examined via molecular dynamic simulations. The nanoparticle diffusion time is larger than the nanosize droplet spreading time. The nanoparticles do not have enough time to diffuse to the vicinity of contact line region; thus, the self-assembly of nanoparticles does not occur. The addition of non-surfactant nanoparticles hinders rather than enhances the droplet spreading kinetics during the nanosecond process. The contact line velocity decreases with increasing nanoparticle volume fraction and particle–water interactions, as a result of increasing surface tension and solid–liquid friction and the absence of nanoparticle ordering in the vicinity of contact line. The structural disjoining pressure is ten times larger than the unbalanced Young's stress, which can facilitate the contact line motion if the nanoparticle self-assembly occurs in the vicinity of contact line region.
3. The surface tension, viscosity, and rheology of gold–water nanofluids were calculated using molecular dynamic simulations which provide a microscopic interpretation for the modified properties on the molecular level. The gold–water interaction potential parameters were changed to mimic various nanoparticle types. The results show that the nanoparticle wettability is responsible for the modified surface tension. Hydrophobic nanoparticles always tend to stay on the free surface, so they behave like a surfactant to reduce the surface tension. Hydrophilic nanoparticles immersed in the bulk fluid impose strong attractive forces on the water molecules at the free surface which reduce the free surface thickness and increase the surface tension of the nanofluid. Solid-like absorbed water layers were observed around the nanoparticles which increase the equivalent nanoparticle radius and reduce the mobility of the nanoparticles within the base fluid which increase the nanofluid viscosity. The results show the water molecule solidification between two or many nanoparticles at high nanoparticle loadings, but the solidification effect is suppressed for shear rates greater than a critical shear rate; thus, Newtonian nanofluids can present shear-thinning non-Newtonian behavior.
4. A mesoscopic study of the nanofluid wetting kinetics using the lattice Boltzmann method was conducted to investigate the effects of nanoparticle motions in nanoscale (10^{-9} m) on the dynamic wetting behaviors that occur in the macroscopic scale (10^{-3} m). The effects of nanoparticle motion in the bulk liquid contribute to the bulk dissipations, which modify the surface tension and the rheology of based fluids. The self-assembly of nanoparticles in the vicinity of the contact line regions contributes to the local dissipations. The effects of nanoparticle bulk and local dissipations on the macroscopic dynamic wetting were studied using mesoscopic simulations. The results show that the LBM is capable to simulate both the microscopic phenomena and the macroscopic

dynamic wetting. Adding hydrophobic nanoparticles facilitates the dynamic wetting, while adding hydrophilic nanoparticles deteriorates the dynamic wetting. The shear-thinning non-Newtonian behavior due to the addition of nanoparticle enhances the dynamic wetting of nanofluids. For the partial wetting droplet, the structural disjoining pressure due to the self-assembly of nanoparticle in the vicinity of contact region enhances the contact line motion. The nanoparticle global deposition has few effects on the dynamic wetting. The study provides multiscale understanding and tunable methods of the nanofluid dynamic wetting.

5. The wetting kinetics of a nanofluid nanodroplet with evaporation on a heated gold substrate were simulated using molecular dynamic simulations. The effects of the initial droplet temperature, substrate temperature, and wettability were examined. The molecule and nanoparticle random motion become significant with the heating conditions, accelerating the nanoparticle diffusion. The nanoparticle sedimentation rate increases with increasing temperature. The nanoparticles tend to deposit uniformly at the bottom of the droplet on the solid surface. The reduction of the liquid–vapor surface tension due to the increasing of substrate temperatures strongly affects the contact line movement for the nanometer water droplet. The effects of evaporation on wetting kinetics are enhanced by the frequency and intensity of water molecule absorption–desorption in the vicinity of contact line region. The initial water droplet temperature had little effect on the contact line motion due to the fast heating process for the nanometer droplet spreading. The substrate wettability affected the spreading much more for spreading with limited evaporation than for spreading with intense evaporation.

7.2 Prospects

As mentioned in Chap. 1, the study of nanofluid dynamic wetting still faces great challenges due to the lack of nanoscale and multiscale experimental techniques and theories. There is still a long way to go in the future before solving these challenges. The present study only draws the branches and trunk in the study of dynamic wetting by nanofluids, and more leaves and flowers are needed to make the trees luxuriant. The prospects of dynamic wetting by nanofluids lie in several aspects, including the nanoscale experimental evidences of nanoparticle self-assembly near the contact line region, theoretical model with combination of the effects of the bulk and local dissipations, and the numerical model with the capacity of simulating sufficient nanoparticle number. One candidate of experimental techniques to detect the self-assembly of nanoparticles near the contact line region is atomic force microscopy (AFM), which has been reported in the detection of nanoscale profile of contact line region. The hybrid of the molecular kinetic theory and the hydrodynamic model could be the potential option to establish the dynamic wetting theoretical model of nanofluids, which can combine the bulk and local dissipations revealed in this study. In the numerical studies, the lattice Boltzmann method is the promising tools in the simulation of dynamic wetting by nanofluids. However, a reasonable colloidal model is still needed in simulating the nanofluids.