NON-EQUILIBRIUM MOLECULAR SIMULATIONS OF SIMPLE FLUID TRANSPORT AT FLUID-SOLID INTERFACES AND FLUIDIC BEHAVIORS AT NANOSCALE

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ABSTRACT

Nanofluidics has shown promising potential for applications that could significantly impact our daily life, such as energy harvest, lab on a chip, desalination, etc. Current techniques to realize nanofluidic ideas are still very limited due to manufacturing technology. Although sub-micron fabrication techniques are undergoing rapid development recently, scientists and engineers are still not able to access actual nanometric systems. This reason prompts the development of computational tools to reveal physical principles underlying nanofluidic phenomena. Among various numerical approaches ranging from macroscopic to microscopic, molecular dynamics stands out because of its ability to faithfully model both equilibrium and non-equilibrium nanosystems by involving an appropriate amount of molecular details. The results from molecular dynamics simulations could elucidate essential physics and benefit designs of practical nanofluidic systems.

This thesis attempts to provide the theoretical foundation for modeling nanofluidic systems, by investigating nanoscale fluid behaviors and nanoscale fluid-solid interfacial physics and transport for simple fluids via molecular dynamics simulations. Boundary-driven-shear, homogeneous-shear and reverse non-equilibrium molecular dynamics methods are implemented to generate non-equilibrium systems. The fundamental fluid behaviors such as velocity profile, temperature distribution and rheological material functions under steady planar shear are explored comprehensively by each method corresponding to different perspectives. The influences of nanoscale confinement are analyzed from the comparison among these methods. The advantages and disadvantages of each method are clarified, which provide guidance to conduct appropriate molecular dynamics simulations for nanofluidics. Further studies on the intrinsic slip of smooth solid surfaces is realized by the boundary-driven-shear method. Inspired by previous hypothesis of momentum transfer, two mechanisms of fluid-solid interfacial friction are studied extensively. The study reveals the physics behind the transition from "defect slip" to "collective slip" when the shear rate is increasing. The thesis ends with the study of effective slip on nanoengineered su-

perhydrophobic surfaces. The observation indicates that even for superhydrophobic surfaces with the same gas fraction, the resulting slip length may vary by orders of magnitude depending on the detailed topography generating either continuous or isolated liquid-vapor interface. The fine variation of the slip length attracts more attention, which is induced by the meniscus curvature effect of the entrapped bubble. The combination of the meniscus curvature effect and the gas fraction dependence provides the possibility to tailor the slip properties on superhydrophobic surfaces and to prompt macroscale drag reduction applications.