

卓越した大学院拠点形成支援補助金  
「流動ダイナミクス知の融合教育研究世界拠点」  
平成 25 年度 博士課程後期学生国際会議派遣 参加報告書

氏名／専攻・学年 Name / Department	Chilukoti Hari Krishna / Department of Nanomechanics
学会名 Conference's name	The 4th International Symposium on Micro and Nano Technology
開催地 Venue (Name of the facility, city & country)	Shanghai International Convention Center, Shanghai, China
日程 Conference period	October 8 <sup>th</sup> to 12 <sup>th</sup> , 2013
発表タイトル Presentation Title	A Molecular Dynamics Study on Effect of Temperature on Diffusion in the Vicinity of an $\alpha$ -quartz Surface/Alkane Interfaces
<p>【発表概要、他の講演等から得られた知見等を記入してください。】 Brief summary of your presentation, what you learned from other presentations, etc.</p> <p>In my paper, molecular dynamics (MD) study has been performed to study structure and transport properties in liquid alkanes contacting various surfaces of silica (<math>\alpha</math>-quartz). MD simulations were used to examine density, self-diffusion coefficient of liquid methane and decane in the vicinity of (001) OH<sup>-</sup> and H<sup>-</sup> terminated silica (<math>\alpha</math>-quartz) surfaces at various temperatures. Methane and decane molecules were modeled by the TraPPE and NERD united atom force fields, respectively. The silica wall was modeled using Lopes et al. force field. Typical hydrophobic and hydrophilic silica surfaces were generated by terminating the surfaces with hydrogen and hydroxyl groups. Adsorption of alkane molecules on both the solid surfaces was observed to be more remarkable at lower temperature. In-plane self-diffusion coefficient of methane and decane liquids in the vicinity of <math>\alpha</math>-quartz substrate was studied at three temperatures. It is observed that self-diffusion coefficient value in the adsorption layer near hydrophobic surface is higher than the value near hydrophilic surface. It is found that diffusion coefficient value in the adsorption layer contacting the solid wall is higher with larger chain length of molecules when they are compared at the same reduced temperature.</p> <p>A study of confined nanoscale molecules has practical importance in researching the lubrication, adhesion, nanotribology and fabrication of nanomaterials. It also has scientific importance in understanding new physics that occur due to finite-size and reduced dimensionality effects. Molecular dynamics simulations of Lennard-jones particles and water were performed in confined slit pores with multibaric-multithermal ensemble method. Self-assembly and polymorphic transitions of surfactant molecules in water within a nanotube and the effect of water-nanotube interactions on the self-assemble morphologies were examined. By adding chemical patterns on the inner surface of nanochannels dynamical properties of the confined surfactants solutions could be</p>	

modified from shear thinning to shear thickening on basis of molecular simulation of confined surfactant solutions.

The orientation of nanotubes suspended in a fluid is nonuniform, the carbon nanotubes will go to random distribution, namely rotational distribution takes place. Knowledge of the rotational diffusion coefficient is important to align the carbon nanotubes so as to control the thermal, optical, electric properties of suspensions. However rotational coefficient is difficult to measure from the experiments. Therefore, equilibrium and nonequilibrium molecular dynamics simulations were developed to obtain the rotational diffusion coefficient. They calculated the rotational diffusion coefficients using the Green-Kubo formula and Einstein relation. However these results are not in good agreement with theoretical predictions.

In semiconductor manufacturing industry, wafer cleaning is important for the final performance of the device. Recent shrinking of the devices expects the wet cleaning process to solve complex problems occur in the cleaning process. However, wet cleaning process involves nanoscale phenomena at the solid-liquid interface. So, molecular dynamics simulations were performed for wetting phenomena at a solid surface with a nanometer-scale slit pore. The effect of solid-fluid interaction strength and slit pore dimension were examined on the wetting phenomena. Time dependent fluid slit pore filling characteristics are dependent on the fluid-solid interaction strength. The local energy state of the liquid molecules in the vicinity of the slit pore becomes lower with the increase of the interaction intensity, which attracted the energy imbalance in the system and the liquid membrane reached the wetting state.