THE CHARACTERISTICS OF THERMAL ENERGY AND MOMENTUM TRANSFER ACROSS SOLID-LIQUID (S-L) INTERFACES BETWEEN FACE-CENTERED CUBIC (FCC) LATICE AND SIMPLE LIQUID

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DECLARATION

I declare that this project report entitled "The Characteristics Of Thermal Energy And Momentum Transfer Across Solid-Liquid (S-L) Interfaces Between Face-Centered Cubic (Fcc) Latice And Simple Liquid" is the result of my own work except as cited in the references

Signature   :   ....

Name   :   ....

Date   :   ....

APPROVAL

I hereby declare that I have read this project report and in my opinion this report is sufficient in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering.

Signature   :   ....

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Date   :   ....

DEDICATION

To my beloved mother and father

ABSTRACT

The transfer of thermal energy and momentum over the solid-liquid (S-L) interface for alkanes liquid, which are typical liquids applied for lubrication, contacting gold (Au) having the Face-Centered Cubic (FCC) structure with two types of crystal planes, (100) and (111) were examined using Non Equilibrium Molecular Dynamics (NEMD) simulations. The influence of the lattice-scale roughness of the solid surface was determined. Two configurations consists of shear system and non-shear system were made. The non-shear system was applied with constant heat flux and different temperatures between two sides of solid walls and liquid alkanes. The two parallel solid walls sliding at a constant speed and in opposite directions caused viscous heating to occur on the liquid for the shear system. The surface layer of solid atoms and first absorption layer was analysed. There is a temperature jump on the shear and non-shear system where the temperature jump measured for the non-shear system was seen to be larger than the shear system. For the shear system, the slip length was examined. The slip length was found to be affected by the surface roughness. The thermal boundary resistance was measured for both setup to understand the characteristic of thermal energy transfer. It was found that the shear system and surface structure influenced significantly the thermal energy transfer at S-L interfaces.

ABSTRAK

Pemindahan tenaga haba dan momentum ke atas (SL) antara muka pepejal-cecair untuk alkana cecair, yang adalah cecair yang biasa digunakan untuk pelinciran, menghubungi emas (Au) mempunyai padu berpusatkan muka dengan dua jenis pesawat kristal, (100) dan (111) diperiksa dengan menggunakan ketidakseimbang molekular dinamik simulasi. Pengaruh kekasaran skala kekisi permukaan pepejal telah ditentukan. Dua konfigurasi sistem ricih dan sistem bukan ricih telah dibuat. Sistem bukan ricih telah digunakan dengan fluks haba tetap dan suhu yang berbeza antara kedua-dua belah dinding pepejal dan cecair alkane. Kedua-dua dinding pepejal selari meluncur pada kelajuan yang tetap dan pada arah yang bertentangan, mengakibatkan alkana cecair yang diluncurkan, menyebabkan pemanasan likat berlaku pada cecair untuk sistem ricih. Lapisan permukaan atom pepejal dan lapisan penyerapan pertama cecair telah dianalisis. Terdapat lompatan suhu pada sistem ricih dan bukan ricih di mana lompat suhu yang telah diukur untuk sistem bukan ricih dilihat lebih besar daripada sistem ricih. Untuk sistem ricih, panjang slip diperiksa. Panjang tergelincir didapati terjejas oleh kekasaran permukaan. Rintangan sempadan termal diukur untuk kedua-dua persediaan bagi memahami ciri-ciri pemindahan tenaga haba. Ia didapati bahawa sistem ricih dan struktur permukaan sangat mempengaruhi pemindahan tenaga haba di antara muka S-L.

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AA	All-Atom
AUA	Anistropic United Atom
EAM	Embedded Atom Model
FCC	Face-Centered Cubic
HPC	High-performance computing
LJ	Lennard Jones
MBR	Momentum Boundary Resistance
MD	Molecular Dynamic
NEMD	Non Equilibrium Molecular Dynamic
OPLS	Optimized Potentials for Liquid Simulations
PBC	Periodic Boundary Conditions
r-RESPA	Reversible Reference System Propagator Algorithm
RESPA	Reference System Propagator Algorithm
S-L	Solid-Liquid
SKS	Siepmann, Karabomi and Smit
TBR	Thermal Boundary Resistance
TJ	Temperature Jump
TraPPE	The Transferable Potentials for Phase Equilibria
UA	United Atom
VJ	Velocity Jump
VLCC	Vapor-Liquid Coexistence Curves

CHAPTER 1

INTRODUCTION

1.1   Background Information

Technology has advanced a lot in the last few decades. Technology sometimes involves a particular piece of apparatus, however that apparatus are often unbelievably straightforward or dazzlingly complicated. It can be anything from the discovery of the wheel, all the way up to laptops and personal computer. The word technology can be described as the science or knowledge that can be used in practice to solve major or minor problems or to invent useful tools to ease our daily lives. Human have achieved a lot with the aid of technology such as people can still keep in touch with their friends, even though the friend is on the other side of the earth and they have cured many diseases that it had never been cured before.

Tribology is one of the oldest technologies in the world. Tribology literally means "the science of rubbing" based on the dictionary. It can be defined as the science and technology of interacting surfaces in relative motion and of related subjects and practices (Bhushan, 1973). Tribology includes studying and applying the principle of friction, lubrication and wear. The knowledge of various disciplines including physics, chemistry, materials science, solid mechanics, fluid mechanics, applied mathematics, thermodynamics, heat transfer, lubrication, rheology, machine design, reliability and performance are required to understand the surface interaction in a tribological interface which is very complicated (Bhushan, 1973). Numerous of research and study regarding tribology has been done which leads to better performance, fewer breakdowns, greater plant efficiency and significant savings. The main purpose of the research in tribology are mainly to minimalize and eliminate losses resulting from friction and wear at all levels of technology that involve with the rubbing of surfaces (Bhushan, 1973).

Lubrication system, which is a field of Tribology is one of the technology that can clearly be seen in everyday life whether directly or indirectly. The lubrication system is one of the oldest technology in the world. It has been introduced for thousand years ago. Lubrication system is the application of lubricant that reduce the frictional resistance and wear or other forms of surface deterioration between two load-bearing surfaces (Ko, 1985). Initially, lubricants were based on olive oil and rapeseed oil, as well as animal fats. Then,

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when the civilization enters the Industrial Revolution, the growth of lubrication accelerated in the Industrial Revolution going along with the use of metal-based machinery (Hsu, 2004). Nowadays, most of the lubrication system are being researched at the molecular scale due to recent development in nanotechnology (A.R. Saleman et al., 2018). Therefore, the study of lubrication at the molecular scale is greatly beneficial for the next generation.

Solid-Liquid (S-L) interface is one of common system in terms of tribology applications for the lubrication system. The typical case for lubrication is when the S-L interface is in the nanometer scale (Abdul Rafeq bin Saleman, Chilukoti, Kikugawa, Shibahara, & Ohara, 2017a). Generally, S-L interface plays an elementary role in numerous fields and the application of the interface is numerous such as batteries, fuel cells, lubricant system or coating system (Streator, 2015). Moreover, S-L interfaces has assists human in various way especially in the industry field. The S-L interface helps with an understanding of the physical phenomena and structural information of the interface, at the atomic scale, for instance in chemical change which is called catalysis, crystal growth, lubrication, chemistry, mixture system, and in several biological reactions (Park & Seo, 2011). In the lubrication system, due to viscous heating, the thermal energy occur from the flow energy in the sheared liquid film. The flow energy, which is a Couette-like macroscopic flow are generated in the sheared liquid film when there is a shear on the two solid surface contacting the liquid with different velocity. Then, the thermal energy increased the temperature of the liquid film and via heat conduction, the increased temperature is transferred over the S-L interface to the solid walls (Abdul Rafeq bin Saleman et al., 2017a). Hence, a good understanding of thermal energy transfer and momentum transfer is important to S-L interfaces and lubrication system.

S-L interface have been frequently studied in order to understand the characteristics of some application. Interfacial thermal resistance is defined as the measurement of thermal resistance between two different surfaces in contact with each other resulting in discontinuity of temperature or drop of temperature at the interface under a heat flux. Numerous of research have been studied regarding the thermal energy transfer and momentum transfer of S-L interface. One of the study that have been done recently are the comparison of the heat transport at S-L interfaces between non-shear and shear (Rafeq et al., 2018). A molecular dynamics simulation, was used for the simulation and the heat flux was measured which were used to determine the thermal boundary resistance (TBR).

For the application like lubrication system, it is important to understand and study the S-L interface that one may give the system more efficient for the future. There are

numerous of research regarding the thermal energy transfer and momentum transfer of S-L interface has been done and explored, but the characteristic of the thermal energy transfer and momentum transfer have not been clearly study. Rafeq (Abdul Rafeq bin Saleman et al., 2017a) has done the investigation of the transfer of thermal energy and momentum over the S-L interface between gold and sheared liquid alkanes. However, the research does not compare between sheared and non-sheared system. Another studies regarding thermal transport has been made by Rafeq (Abdul Rafeq bin Saleman, Chilukoti, Kikugawa, Shibahara, & Ohara, 2017b). The study was on a molecular dynamics study on the thermal transport properties and the structure of the solid–liquid interfaces between Face-Centered Cubic (FCC) crystal planes of gold in contact with linear alkane liquids. The study examined the influences of the lattice-scale roughness of the solid surface in contact with the liquid but it is only based on the thermal transport and the momentum transfer was not considered. The lattice-scale roughness of solid surface in terms of the characteristic of thermal energy and momentum transfer with shear system and non-shear system have yet to be clarify.

Furthermore, Rafeq (Rafeq et al., 2018) have investigated the comparison of the heat transport at S-L interfaces between non-shear and shear systems. From his study, the heat transport characteristics at S-L interfaces were found to be significantly influenced by the shear system and solid wall surface structure. However, the study only focus on the heat transport, while the momentum transfer was not considered.

1.2 Problem Statement

It is crucial to know characteristic and the influences of thermal energy and momentum transfer in order to know which material is better in providing a better lubricant for a better future. This project will study the characteristic and the influences of thermal energy and momentum transfer across the S-L interface. The transfer of thermal energy and momentum over the S-L interface for alkanes liquid, which are typical liquids applied for lubrication, contacting gold (Au) having the Face-Centered Cubic (FCC) structure with two types of crystal planes, (100) and (111). The influence of the lattice-scale roughness of the solid surface on thermal energy and momentum transfers at the S-L interface will be examined using Non Equilibrium Molecular Dynamics (NEMD) simulations.

1.3   Objective

Therefore, based on the problem statement which have been describe above, the objective of this research is:

- To identify the characteristics of the transfer of thermal energy and momentum over the solid-liquid interface for simple liquid.
- To clarify the influences of the lattice-scale roughness of solid surface on the characteristics of thermal energy and momentum transfer.

1.4   Scope

The scopes are identified based on the objectives of this research. The 2 Face-Centered Cubic structure with two types of crystal plane which is (100) and (111) will be used in this study. A single liquid alkane (methane) or simple liquid is chosen. The simple liquid are linear liquid and not lengthy molecule. The thin liquid is sandwiched between two parallel solid walls where the liquid alkane is put between two solid walls which is gold (Au). The factor that will be measured in this research on the S-L interface are density, temperature, heat flux, slip length and the thermal boundary resistance. A Non Equilibrium Molecular Dynamics simulation will be used in this study. The Reversible Reference System Propagator Algorithm (r-RESPA) method with multiple time steps will be used. Two setup of simulation will be made in this study that is non-shear system that and shear system. The non-shear system consists of different temperature; both side of the solid wall are set at low temperature while the liquid at the center is set at high temperature while for the shear system, a constant speed is applied for both of the solid wall in the opposite direction.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter illustrate the literature review from the past about the S-L interface in details. It consists of the criteria that need to be added in studying the characteristic in terms of thermal energy transfer and momentum transfer such as molecular dynamic simulation, simulation model system, the potential function, the thermodynamics properties and measurement method for density, temperature, momentum and heat flux and thermal boundary resistance and momentum boundary resistance.

2.2 Molecular Dynamic Simulation

Molecular Dynamic (MD) simulation is a technique for calculating the equilibrium and transport properties of particle systems. The first simulation was in the 1960s where the model molecules represented by a continuous potential were carried out using MD. In 1964, Rahman (A., 1964) was the first one who calculated the diffusion coefficient in a argon atoms system interacting through a Lennard-Jones potential using MD (Ewen, Heyes, & Dini, 2018).

It is stated that molecular dynamic serves two roles. First, the solutions of the equations of motion for times comparable with the correlation times of interest need to be essentially exact, so that we may accurately calculate time correlation functions. Second, the use the method to generate states sampled from the microcanonical ensemble (Tildesley, n.d.). An ensemble is commonly a probability distribution for the state of the system (Ewen et al., 2018). The microcanonical also called NVE ensemble due to the total number of particles, N, the volume of the system, V and the total energy in the system, E, remain constant.

The Non-Equilibrium Molecular Dynamics (NEMD) simulation is based on time-reversible equations of motion (Wm.G.Hoover, 2005). The first NEMD simulation were perform in 1970s which imposed shear flows at large shear rates. Until 1970s, NEMD simulations were quasi-2D where they used periodic boundary conditions (PBC) in only two

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directions. Then, equations of motion for imposing shear flow in system which PBC in all three Cartesian direction were created in 1980 (Ewen et al., 2018).

A number of facet must be have been thought about carefully, from the inherent limitation of the time and length scales that can be modelled to the accuracy of the representation of the intramolecular and intermolecular interactions in order for NEMD simulation to be useful in terms of predictive capabilities (Ewen et al., 2018). The computer hardware and software available, the system size, as well as the complexity of the force-fields used are the factors that will decide the computational time required to conduct MD simulations.

Classical MD force-fields require a time step of approximately 1 femto second (fs) to ensure energy conservation (Tildesley, n.d.). This means that even when performed on multiprocessor high-performance computing (HPC) systems using highly parallel MD software, only ns or μs time scales can be accessed in MD simulations in extreme cases, since they correspond to millions / billion timescales (Ewen et al., 2018). The main consequence of the short accessible time scales in NEMD simulations where shear is applied is that relatively high shear rates are required to ensure that the properties of interest reach a stable state (generally $> 10^7 s^{-1}$) (Bair, McCabe, & Cummings, 2002; Bair, McCabe, McCabe, Cummings, & Cummings, 2002). The ability to simulate lower shear rates was a long-term objective of NEMD simulations to facilitate direct overlap with experiments and real components (Ewen et al., 2018).

2.2.1 Simulation System

In MD simulation, there are several simulation system that have been used to study the S-L interface. Numerous of numbers have been studied for the system that consists of a liquid film confined between two parallel solid walls (Khare, Keblinski, & Yethiraj, 2006; Taku Ohara & Torii, 2005; Rafeq et al., 2018; Abdul Rafeq bin Saleman et al., 2017a, 2017b; Soong, Yen, & Tzeng, 2007; Torii, Taku Ohara, & Kenji Ishida, 2007). One of the study used this simulation system to clarify the influence of interaction between solid and liquid molecules and the spacing of molecular alignment on the surface of the solid wall (Torii et al., 2007). It is found that in order to analyse thermal energy flux across the system, many research set the temperature of the left solid wall higher than the right one which it can produce thermal energy flux (Abdul Rafeq bin Saleman et al., 2017b).

Another study has been made on same simulation system on comparing the shear and non-shear system (Rafeq et al., 2018). In the study, two setup have been made to compare the non-shear and shear system, that is the center of the liquid was set at high temperature while both of the solid walls was set at low temperature which is for the non-shear system and for the shear system, a shear was applied on both solid walls with the same speed in the opposite direction with the different temperature setup that was applied on the non-shear system simultaneously. There were numbers of studies that used the shear system at S-L interface to examine the momentum transfer that used the same simulation system (Khare et al., 2006; Taku Ohara & Torii, 2005; Abdul Rafeq bin Saleman et al., 2017a). By using the simulation system that have been describe above, it is observed that the simulation system helps to analyse on the momentum transfer clearly.

2.2.2 Potential Function

Potential function is one of the important factor before starting the simulation. In general, the potential energy is described by pair potentials. The potential energy is usually described by pair potentials. The potential energy contains the interesting information regarding intermolecular interactions. The predictions made by using either analytical equations of state or molecular simulation are only as accurate as the underlying models they employ (Eggimann, Siepmann, & Fried, 2007). Models that make use of transferable parameters are one option for supplementing the low levels of experimental data available for high temperature or high pressure systems. For example, the similar parameter are fitted to be accurate at several state points, including those beyond constraints of the initial parameterization conditions. In general, the potential energy is described by pair potentials.

2.2.2.1 Liquid

In the past, there were three types of common model used to replicate linear alkane liquid namely the united atom (UA) model, the anisotropic united atom (AUA) model and the all-atom (AA) model. The UA model is a good approximation for simulating molecular systems in which the intermolecular motion is much more important than the intramolecular motion. In addition, the UA model was utilized in most recent simulation system where carbon and hydrogen atoms were gathered in as a single interaction site represented as a pseudoatom (Marcus G. Martin and J. Ilja Siepmann, 1998; Taku Ohara, Yuan, Torii, Kikugawa, & Kosugi, 2011; Rafeq et al., 2018; Abdul Rafeq bin Saleman et al., 2017b,

2017a). The UA model are found to be useful for a quantitative understanding of the dynamic behaviour of medium sized alkanes (Mondello & Grest, 1995). Furthermore, UA model capable of quantitatively predicting the adsorption properties of both linear and branched alkanes responsible for neutral molecular sieves (Dubbeldam et al., 2004). The AA model replicates all the atoms in a molecule that made the computation time in a simulation is longer. Every atom is regarded as an individual interaction site in AA model (Guevara-Carrion, Hasse, & Vrabec, 2012). In the AUA model, hydrogen and carbon atoms are grouped in a single interaction site, but a certain distance from the carbon atom is displaced at the center of the force to better account for the presence of the hydrogen atoms (Ungerer et al., 2000).

Marcus (Marcus G. Martin and J. Ilja Siepmann, 1998) stated that there are three united-atom force field; optimized potentials for liquid simulations (OPLS), Siepmann, Karabomi and Smit (SKS) and The Transferable Potentials for Phase Equilibria (TraPPE). The OPLS united atom model was parametrized using isobaric – isothermal Monte Carlo simulations to provide accurate liquid density vaporization heats for short alkanes at atmospheric pressure (Jorgensen & Swenson, 1984). It contains different LJ parameters for the methyl group in ethane, the methyl group in all other n-alkanes and the methylene group. For SKS, Monte Carlo in the Gibbs ensemble was subsequently used to calculate the vapor-liquid coexistence curves (VLCC) of n-alkanes. It used the same LJ diameter, but different magnitude if well depth, to account for methyl and methylene group. Previous study has found that OPLS force-field overestimate the critical temperature of n-alkanes and SKS force-field overestimated the critical temperature of the shorter n-alkanes. The researcher stated that TraPPE models have been shown to be reasonably accurate for several systems beyond the state points and molecules used in the parameter fitting (Eggimann et al., 2007). Molecular interactions in the TraPPE force-field using UA model are described by pairwise-additive Lennard-Jones (LJ) and Coulomb potentials for the non-bonded interactions.

Based on previous studies, most of the investigation use a similar model system regarding to the model systems. For the CH_4 liquid, the UA model are used as the model where carbon and hydrogen atoms were assembled in as a single interaction site represented as a pseudoatom that has been mentioned on the above. It was then modelled by using Transferable Potential for Phase Equilibria (TraPPE) force field (Abdul Rafeq bin Saleman et al., 2017a).

2.2.2.2 Solid

As for the solid walls, there are three common potential function used to replicate metal solid, namely Morse potential, Lennard Jones (LJ) potential and embedded atom model (EAM). For LJ potential, it is the most commonly used interaction model. An attempt was made to parameterize the potential of LJ for metals but no practical application has been found.

The EAM is a many-body potential used for a wider range of metals. Numbers of study has used the EAM model in their research. One of the earlier studies showed that the EAM model provides a good description of gold (Au), copper (Cu), palladium (Pd), silver (Ag), platinum (Pt), nickel (Ni), aluminium (Al) and some of the alloys (Foiles, Baskes, & Daw, 1986). A Morse potential was first proposed by Philip M. Morse in 1929 (Morse Philip M., 1929). Moreover, it was popular potential for simulation of metals that have face centered-cubic and hexagonal close packed structures and it can also be used to study the atomic properties of metals (Girifalco & Weizer, 1959). Similar to Lennard-Jones, but more bonding and better suited for cases where attractive interaction results from the formation of a chemical bond (Zhigilei, 2013).

2.2.3 Numerical Integration Method

It is obvious that a good algorithm to integrate Newton's equation of motion is required for a better MD simulation. The process of integrating the equation of motion can be achieved by using several kinds of algorithm. In the MD simulation, the Newtonian equation of motion decide the movement of the atoms included in molecules. The speed of an algorithm is not really significant due to the small fraction of time spent on integrating the equation of motion. The accuracy of the large time step is more important because the longer the time step, the less force evaluation per unit of simulation time is required. Therefore, it is advantageous to use a sophisticated algorithm that use a long time step (Daan Frenkel; Berend Smit, 1996).

A variety of techniques were introduced to increase the time in molecular dynamic simulations in an attempt to overcome these difficulties. According to Benedict J. Leinkuhler (Leimkuhler, Reich, & Skeel, 1996), there are four categories consists of the numerical integration methods that can be describe based on their way of handling the components of linearized dynamics. The first method are the method that accurately resolve the highest