THE THERMAL ENERGY TRANSFER ACROSS SOLID-LIQUID INTERFACES OF METHANE AND 111 FACE CENTERED CUBIC (FCC) SURFACE FOR ULTRA THIN LIQUID FILM THICKNESS

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A report submitted in partial fulfilment of the requirements for the degree of Bachelor of Mechanical Engineering

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DECLARATION

I declare that this thesis entitled “The thermal energy transfer across solid-liquid interfaces of methane and 111 face centered cubic (fcc) surfaces for ultra thin liquid film thickness is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree. The work contained in the report is original and has been done by me under the general supervision of my supervisor.

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Name : .....

Date : .....

APPROVAL

I hereby declare that I have checked this report entitled “The thermal energy transfer across solid-liquid interfaces of methane and 111 face centered cubic (fcc) surfaces for ultra thin liquid film thickness” and in my opinion, this thesis it complies the partial fulfillment for awarding the award of the degree of Bachelor of Mechanical Engineering with Honours

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DEDICATIONS

I dedicate my thesis to everyone who kept my success in their prayers.

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ABSTRACT

The thermal energy transfers over the two confined solid walls with an ultra thin liquid film placed between them were investigated. The study on solid-liquid (S-L) interface have been found in several engineering applications such as lubrications and coatings. In the past there are a number of study that look into thermal energy and momentum transfer, however the influence of ultra thin liquid film thickness on the thermal boundary resistance has yet to be explored. The methane alkane liquid was examined as ultra – thin film with the thickness of 60 Å, 30 Å and 10 Å to study the influence of the thickness of liquid film on the thermal energy transfer. The method applied in the simulation model for this system is Reversible Reference System Propagator Algorithm (r-RESPA). The characteristics of thermal boundary resistance (TBR) at the S-L interfaces are evaluated based on the temperature jump (TJ) and heat flux at the interfaces. It is found that the value of the heat flux is correlated to the temperature jump (TJ) as it increases along the reduction of the liquid film thickness. The thermal boundary resistance (TBR) is found in inverse correlation with the TJ and the heat flux. The obtained result shows that the liquid film thickness influences the heat transfer at the S-L interface.

ABSTRAK

Pemindahan tenaga haba ke atas dua dinding pepejal terkurung dengan filem cecair ultra nipis yang diletakkan di antara mereka disiasat. Kajian mengenai antara muka pepejal-cecair (S-L) telah dijumpai dalam beberapa aplikasi kejuruteraan seperti pelinciran dan pelapis. Pada masa lalu terdapat sejumlah kajian yang mengkaji pemindahan tenaga termal dan momentum, namun pengaruh ketebalan filem cair ultra tipis pada rintangan sempadan termal masih belum diterokai. Cecair metana alkana diperiksa sebagai filem ultra tipis dengan ketebalan 60 Å, 30 Å dan 10 Å untuk mengkaji pengaruh ketebalan filem cair pada pemindahan tenaga terma. Kaedah yang diterapkan dalam model simulasi untuk sistem ini adalah Algoritma Propagator Sistem Rujukan Reversibel (r-RESPA). Ciri-ciri rintangan had termal (TBR) pada antara muka S-L dinilai berdasarkan lompatan suhu (TJ) dan fluks haba pada antara muka. Didapati bahawa nilai fluks haba berkorelasi dengan lonjakan suhu (TJ) sepanjang pengurangan ketebalan filem cecair. Rintangan had terma (TBR) dijumpai dalam korelasi terbalik dengan TJ dan fluks haba. Hasil yang diperoleh menunjukkan bahawa ketebalan filem cecair mempengaruhi pemindahan haba pada antara muka S-L.

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CHAPTER 1

INTRODUCTION

1.1 Background

The interfaces of solid and liquid are developing in many technology fields which includes energy materials, electrochemistry, corrosion, catalysis, geochemistry, self-assembly-based biosensors and biological membranes. Interfaces consist of a liquid interposed between solid walls in accurate adjacency are common in small-scale devices. In many cases, the liquid recommends large and undesired adhesive forces. [1]

In the previous studies solid-liquid (S-L) interfaces and hydrocarbon plays an important role in tribology applications related to coating, lubrication, wear and friction[2]. The common chemical structure of hydrophobic is a hydrocarbon motif. The CH bond is only weakly polarized. With the advance of monolayer technology, nowadays it is possible to cover a great variety of surfaces such as different metals and vitreous glass, with a sheet of hydrophobic alkane chains. Other hydrophobic materials are graphite, hydrogen-terminated diamond, and fluorinated hydrocarbons [3].

The alkane liquid was located between the couple solid walls where it slides at steady speed and in adverse directions, that create viscous heating in the liquid. The amount of shear to the liquid and the heat conduction in the method maybe articulate in term of the transfer of thermal energy at the S-L interfaces, individually. In a method of S-L interface, clip will exist used to the liquid when the solid to the liquid will exist move down at different speed. Then thermal energy results in an increase in temperature of the liquid film and will exist moved over the S-L connect to the dependable obstruction by way of heat conduction. The phenomena in the sheared thin liquid film when the liquid film will be in the nanometer scale, that will happen a typical case in lubricating applications, happen difficult on account of further authority of the building of the stable surfaces and the intensely big cut rates. The thin liquid film will exist joint by affecting the dimensional divider at fixed and alike speed in the opposite directions. As a result of cut likely to the thin liquid film, viscous heating will come from at the center of the system, that will exist understand by an increase in temperature of the liquid as far as it reaches a constant state.

Molecular Dynamics (MD) are investigated in the previous study by [4]. MD is used to study the structure and interface diffusion at the interface bounded copper and liquid aluminum. Molecular dynamic simulation occurs a method to pretend the motion of atoms and particle under predefined conditions. MD simulations can then be used to study dynamical processes at the nanoscale and to measure under abroad range of real estate, such as phase spread cooperative, or various reaction functions, further static quantities being radial classification functions and management numbers.

Thermal rectification exists an aspect that heat happen conducted surely in individual direction but harder in the opposite management. An attention in contact the thermal rectification effect exist resolve by calculating the thermal boundary conductance (TBC) at the S-L connect. Thermal rectification maybe entitles the differences in the TBC at the connect between two together opposite heat flow directions; one exists from the liquid to dimensional and vice versa [5]. Different face-centered cubic of gold along the surface of 100, 110 and 111 crystal planes contacting liquid CH_4 exist checked by utilizing non-equilibrium microscopic movement simulations. The examination in contact the warm improvement effect was act by measuring the warm boundary conductance (TBC) at the stable-liquid interface. The results suggest that the factors that influence the warm improvement at the continuous-liquid connect happen the importance of the adsorption of liquid smallest part and the surface form of the complete walls that differ considerably with the three types of crystal planes.

In the completed studies of solid-liquid interfaces [6], they have come up with many new method such as modified surface and synergy between solid and liquid. However, the impact of the reduced temperature and the type of liquid molecules on the thermal energy transfer characteristics at the interfaces has to be investigated. So far in the earlier, the effect of reduced temperature on thermal energy transfer at solid-liquid interface has not been fully understood. Therefore, the purpose of this study is to specifically investigate the characteristics of thermal energy transfer in the molecular scale at the solid-liquid interfaces between face-centered cubic (FCC) lattice of 110 crystal structures and simple liquid at different reduced temperature of liquid. The characteristic of heat energy transfer at solid-liquid interfaces will be evaluated based on the density, temperature, and thermal boundary resistance (TBR) at the interfaces.

1.2 Problem Statement

Thermal energy transfer over solid-liquid interfaces have been tremendous studies in the past, that look into the wettability or interaction of liquid and solid and type of surface structure [7]. Nevertheless, the influences of the thickness of the thin liquid film on the thermal energy transfer across the solid-liquid interfaces have yet to be investigated. Thus, in the present study we would like to look into the influences of thickness of liquid film on the characteristics of thermal energy transfer. The influences of the thickness of the liquid film and the surface structure characteristics will be evaluated in this study.

1.3 Objective

There are two main objectives in this study which first to identify the influences of the extremely thin liquid film on the characteristics of thermal energy transfer second to identify the influences of 111 crystal structure on the thermal energy transfer at solid-liquid interfaces.

1.4 General Methodology

The project progress flows have been planned as shown in figure 1-1. The general progress started with the title selection which is the thermal energy transfer across the solid-liquid interface of methane and 111 face centered cubic (fcc) surfaces for ultra thin liquid film. Related journals were analyzed to understand more on the findings on this study. r-RESPA method will be used in this study to analyze the thermal boundary resistance.

1.5 Scope of Project

Face-centered cubic of 111 with simple liquid of methane, CH_4 is being investigated in this solid-liquid interface. Liquid film thickness of 60 Å, 30 Å and 10 Å which sandwiched between two parallel solid walls is designed to measure on the thermal boundary resistance at the solid-liquid interfaces. Looking into the thermal boundary resistance in relation to the thickness of thin liquid films and the constant heat flux applied across the simulation system without shear.

1.6 Flow chart

This flow chart is the summarized work progress for this present study.

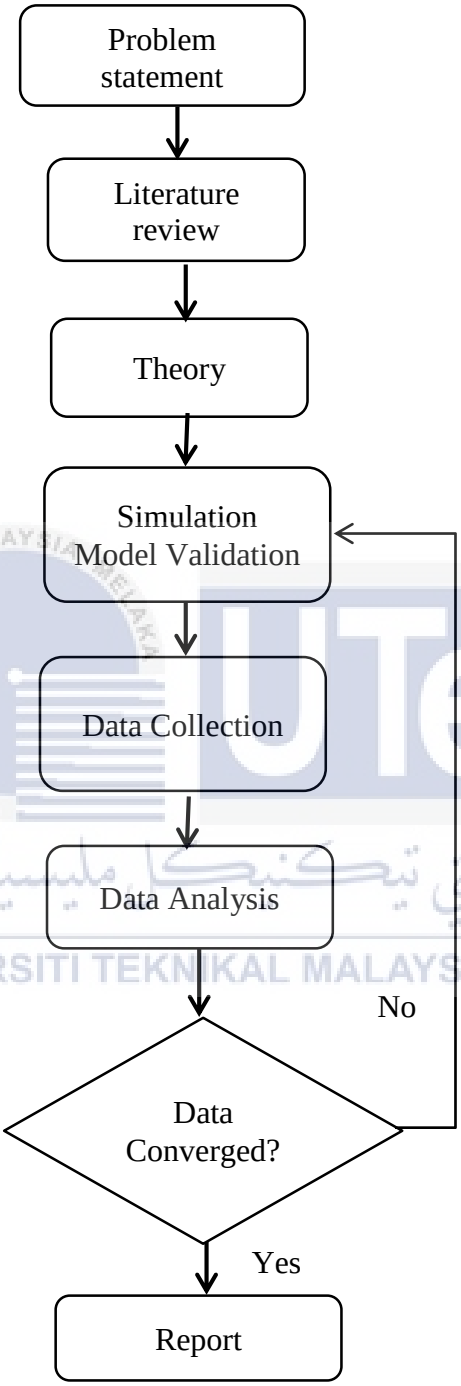


Figure 1-1: Molecular dynamic simulation flow chart

CHAPTER 2

LITERATURE REVIEW

Overview

This chapter will be discussed about the evolution of Molecular Dynamic simulation by using varies type of method. The method applied in the simulation for this project is r-RESPA. This method can be used to calculate the molecular dynamics of the lattice structure during the simulation's analysis.

2.0 Theory of molecular dynamic (MD) simulation

Molecular Dynamics (MD) imitation exist individual of a common plan to study the perceptible nature of method by following the evolution of system which controls organization at the subatomic scale. This models possessions of a scheme of interacting piece by uniformly manipulative the smallest part of something connect between it and make the equating of motion. Combining statistical mechanics and energetic theory, almost undetectable characteristic of ruling class perhaps calculated.

In section 2.1, algorithm of molecular dynamic is about the study of the basis theoretical algorithms in numerical integration. Numerical integration algorithms are integrated such as Verlet algorithm, Leap-frog algorithm, Velocity Verlet algorithm, Beeman algorithm and reversible reference system propagator(r-RESPA) algorithm and dedicated to study both advantages and disadvantages of these algorithms and to improve and develop new numerical integration algorithms on this basis.

In section 2.2, explains about the thermostat and barostat in the molecular dynamic simulations commonly known as algorithm. The most frequently used thermostat algorithm are based on the rescaling of the atomic velocities, and the Berendsen thermostat is the most widely employed for that purpose followed by nose thermostat, nose-hoover thermostat, velocity scaling method and Andersen barostat.

In section 2.3, the potential function explain the method used in molecular dynamic simulation to study on the solid and liquid surface to understand of the findings. In section 2.4, is on the interfacial resistance. In section 2.5, the theory of thermal boundary resistance is explained in details. Section 2.6 briefly explains the solid-liquid interface where section 2.7 on the measurement explains on the density distribution, velocity distribution and heat flux measurement of this solid-liquid interface study.

2.1 Algorithm of Molecular Dynamics

The molecular dynamics algorithm is commonly use today. There are numerical algorithms that have been developed for integrating the equations of motion such as verlet algorithm, velocity verlet, algorithm, beeman's algorithm and leap-frog algorithm.

The microscopic action algorithm common present can even have happen famous to Newton. Nonetheless, the last decennium has visualized a very quick happening contemporary our understanding of integration method, an expected review and a book compile the present state of the field. The algorithm integration differs in the used of every system which examine the movement and the position of the particle and the trajectory files. The trajectory file stores the characteristics of the particle position, velocities and accelerations which works vary with respect to time.

2.1.1 Verlet Algorithm and Velocity Algorithm

Verlet Algorithm is frequently used to calculate trajectories of particles in MD simulations and computer graphics [9] and it happen a mathematical system used to merge equating of motion. In MD simulations, the fundamental to determine numerically the equations of motion for a multi body system composed of interacting particles. Velocity-Verlet invention exist a second-order integrator that working now the excellent most of MD simulations as long as appeal cohesion and extraordinary balance. Verlet invention happen able to perform well to reach an extreme level of precision or correctness accompanying essential number of force evaluations per period step [9]. Equation 2-1 shows the velocity verlet algorithm equation

where *r* the position is, *v* is the velocity, *a* is the acceleration and *t* is the time. δt is known as the time step.

$$r(t + \delta t) = r(t) + v(t)\delta + \tfrac{1}{2}\, a(t)\delta^2$$

$$v(t + \delta t) = v(t) + \tfrac{1}{2}\,[\, a(t) + a(t + \delta t)]\delta t \quad [9]$$

Equation 2-1: The velocity verlet algorithm

Algorithm of high orders can also be derived in a similar method. The Verlet is the one and only algorithms do reduce the number of force evaluations per time step. In the previous study by [10] proved that the Velocity-Verlet (VV) algorithm is more efficient than the typical Steepest descent (SD) algorithm, which is easier to switch between different modes of operation ,energy reduction process and annealing process in a microcanonical ensemble, and requires only one extra empirical parameter ω and storage of the coordinates at the previous time step.

2.1.2 The Leap-Frog Algorithm

Leapfrog Algorithm or integration is a method for numerically integrating differential equations. In the previous study by [11] explains Leapfrog algorithm which is particularly suited for simulations because it is simple, and it can be said as global stability. Leapfrog integration is corresponding to observe positions and velocities at extent of time, startle as if it "leapfrog" over one another. Leap Frog method is generally useful in solving the equation of motion of a dynamical system in classical mechanics. The *r* is the position, v exist the velocity, a is the acceleration and t is the time as in the equation stated in Equation 2-2. δt is known as the time step.

$$r(t + \delta t) = r(t) + v(1 + \tfrac{1}{2}\,\delta t)\,\delta t$$

$$v(t + \tfrac{1}{2}\,\delta t) + v(t - \tfrac{1}{2}\,\delta t) + a(t)\,\delta t \quad [11]$$

Equation 2-2: The leapfrog algorithm

Here it is important to mention the two primary strengths of Leapfrog Scheme when applied to mechanic problems. The first is the time-reversibility of the Leapfrog method where we can calculate the solution in forward δt time steps, and then reverse the direction of integration and can obtain the solution in backwards δt time steps to arrive at the same starting time. The second strength is that the scheme conserves the energy of dynamical systems, a slight change is possible. Particularly, this strength becomes important when computing orbital dynamics.

2.1.3 Beeman's Algorithm

Beeman's Algorithm is a strategy for mathematically integrating conventional differential conditions of order two, all the more explicitly Newton's equation of motion $\ddot{x}=A(x)$. It was intended to permit high quantities of particles in re-enactments of molecular dynamics. There is an immediate or express and an understood variation of the strategy. This calculation is firmly identified with the Verlet algorithm. The benefits of this calculation are that it gives a more precise articulation to the speeds and better energy protection. Equation 2-3 shows the equation of Beeman's algorithm which are is closely related to the verlet integration but the velocities are more accurate where r is the position, v is the velocity, α is the acceleration and t is the time. δt is known as the time step.

$$r(t + \delta t) = r(t) + v(t)\delta + 2/3a(t)\delta t^2 - 1/6a(t - \delta t)\,\delta t^2$$
$$v(t + \delta t) = v(t) + v(t)\delta t + 1/3a(t)\delta t + 5/6a(t)\delta t - 1/6a(t - \delta t)\,\delta t \quad [12]$$

Equation 2-3: Beeman's equation

The algorithm happen described as though admit extreme numbers of atom in MD simulation. It uses a direct or specific and an inherent design.

2.1.4 Reversible reference system propagation algorithm (r-RESPA)

In the previous study on the thermal transport properties on the structure of the solid–liquid interfaces by [6] explains the time integration which was performed using r-RESPA method with multiple time steps. One femto-second (fs) and 0.2 fs integration time steps were used for

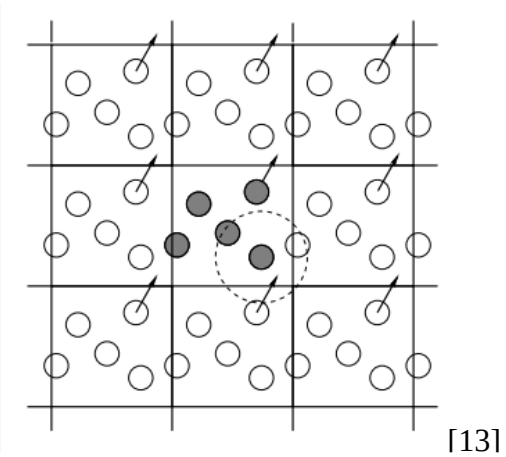
the intermolecular motions and intramolecular motions, respectively. After the system attain the point temperature, it exists equilibrated for 1–4 million period steps practicing speed measure plan, just before the system gained by personal exertion a uniform temperature at 0.7Tc.

The short range force equation defines the time step to be used in a molecular dynamics calculation. The force agreement in equating are naturally non-aligned functions of the distance r_{ij} in the middle pairs of atoms and grant permission happen either complete or short-range in nature. For long-range forces, in the way that Coulombic communication in a classic reliable or concerning life order, each smallest part of something communicate among all possible choice.

Numerical reversible integrators called r-RESPA are the most suitable and best algorithm among the listed above that leads to large speedups in create molecular dynamics course accompanying no loss of efficiency r-RESPA method expected used in molecular dynamics simulations beside polarizable potentials establish induced dipole importance.

2.1.5 Periodic boundary condition

Periodic boundary conditions empower us to mirror a boundless system by treating a generally little part of the system to accomplish a sensible portrayal of the infinite system. The particles of this minor subsystem are constrained by a bunch of limit conditions called a unit cell. During the reenactment, particles are allowed to move in the central cell, consequently, their periodic pictures of the adjoining cells move in an identical manner. This implies any molecule that crosses one limit of the cell, will return on the contrary side. The unit cell of the system is in the middle cell. The possible energy of the framework incorporates communications between this middle cell and its periodic picture. Figure 2-1 shows the periodic boundary conditions as an atom moves exhausted the imitation boundary, a figure piece moves consumed change it. In calculating atom interplay inside the cutoff range, two together genuine in existence and representation neighbours happen included[13].



[13]

Figure 2-1: Periodic boundary condition

First happen that the treatment of demonstrative particles crossing the boundary surfaces of the component, and second is that the calculation of interaction energies or forces accompanying in essence atom being within the copy part. First happen that the situation of active particles crossing the boundary of the component, and next exist that the judgment of interplay energies or force accompanying in essence atom being inside the copied unit.

2.1.6 Ensemble

An ensemble maybe an intensely big accumulation of microscopically writing states of a scheme accompanying sure nonstop visible characteristic [14]. In MD simulations it's used to achieve determinable effect secondary differing thermodynamic environment for realistic models that happen parameterized to review a picked molecular or atomic structure accompanying a particular scope of authenticity. It exists of movable limit for microscopic second-part commonly at the atomistic level. Generally, Microcanonical ensemble (NVE), Isothermal-isobaric ensemble (NPT) Canonical ensemble (NVT), and any additional generalized collection happen make use of in MD imitation. Microcanonical Ensemble (NVE) maybe a method entirely private from changes in volume (V) bear the determined number of piece (N) and Energy (E). An action accompanying no heat exchange exist similar the NVE ensemble [15]. Within the ensemble, the exchange of energetic and P.E. accompanying total strength happen in addition to visualize. Canonical Ensemble (NVT) bear volume (V), particles (N) accompanying a contact of warmth bath accompanying constant temperature (T). Hence, it's in addition to apply as Constant Temperature Molecular Dynamics (CTMD). The strength