Faculty of Mechanical Engineering

THE INFLUENCE OF LIQUID FILM THICKNESS ON THE HEAT TRANSFER AT SOLID-LIQUID INTERFACES

Jannatul Al-Qashah bin Muhammad Ali Jinnah

Master of Mechanical Engineering (Automotive)

2020

THE INFLUENCE OF LIQUID FILM THICKNESS ON THE HEAT TRANSFER AT SOLID-LIQUID INTERFACES

JANNATUL AL-QASHAH BIN MUHAMMAD ALI JINNAH

A report submitted in fulfilment of the requirements for the Master of Mechanical Engineering (Automotive)

Faculty of Mechanical Engineering

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2020

DECLARATION

I declare that this project report entitled "The Influence of Liquid Film Thickness on the Heat Transfer at Solid-Liquid Interfaces" is the result of my own work except as cited in the references.

Signature : ……………………………………………

Name : ……………………………………………

Date : …………………………………

SUPERVISOR 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 Master of Mechanical Engineering (Automotive)

Signature : …………………………………………

Supervisor's Name: …………………………………………

Date : ………………………………………

DEDICATION

Special dedication to my beloved father, mother and sister for their everlasting love and support. This thesis had been done during Malaysia MCO 2020 due to Covid-19 virus.

ABSTRACT

Solid liquid (S-L) interface had been widely used in various industries. Many previous researcher had study the effect of thermal energy transfer across solid-liquid interface. However the effect of difference thickness of thin liquid film and thermal energy transfer had not been study in detail yet. Hence the objective of this report is to investigate the influence of difference liquid film thickness on the thermal energy transfer at solid-liquid interface by using molecular dynamic (MD) simulation. In this report the solid gold (Au) had been choose as two parallel solid walls where liquid methane (CH_4) will be place between them. The simulation test is focusing on the effect of (110) crystal plane only to the thermal energy transfer across the simulation system. The model consists of solid wall and liquid film will be described after the study had been made. The heat flux will be applied constantly from the centre to the both left and right side of the system. The structural quantities such as density distribution, temperature distribution and heat flux will be calculated during this test. The thermal boundary resistance (TBR) will be used to describe the characteristic of thermal energy transfer at S-L interface of the simulation system. The result show that the value of TBR decrease when the thickness of think film increase. Besides, the number of molecule will also affect the TBR value. When the number of molecule decrease the value of TBR will be decrease which will lead to increasing the amount of thermal energy transfer.

PENGARUH KETEBALAN FILEM CECAIR PADA PEMINDAHAN HABA PADA ANTARA MUKA PEPEJAL-CECAIR

ABSTRAK

Antaramuka cecair pepejal (S-L) telah digunakan secara meluas dalam pelbagai industri. Banyak penyelidik terdahulu telah mengkaji kesan pemindahan tenaga terma di antara muka pepejal-cecair. Walau bagaimanapun, kesan perbezaan ketebalan filem cecair nipis dan pemindahan tenaga haba belum dikaji secara terperinci. Oleh itu objektif laporan ini adalah untuk mengenal pasti pengaruh perbezaan ketebalan filem cecair pada pemindahan tenaga termal pada antara muka pepejal-cecair dengan menggunakan simulasi dinamik molekul (MD). Dalam laporan ini emas padu (Au) telah dipilih sebagai dua dinding pepejal selari di mana metana cair (CH "CH"〗 _"4") akan berada di antara mereka. Ujian simulasi memfokuskan pada kesan (110) satah kristal hanya terhadap pemindahan tenaga termal di seluruh sistem simulasi. Modelnya terdiri dari dinding padat dan filem cair akan digambarkan setelah kajian dibuat. Fluks haba akan digunakan secara berterusan dari pusat ke kiri dan kanan sistem. Kuantiti struktur seperti taburan ketumpatan, taburan suhu dan fluks haba akan dikira semasa ujian ini. rintangan had terma (TBR) akan digunakan untuk menggambarkan ciri pemindahan tenaga terma pada antara muka S-L sistem simulasi. Hasilnya menunjukkan bahawa nilai TBR menurun apabila ketebalan filem berfikir meningkat. Selain itu, bilangan molekul juga akan mempengaruhi nilai TBR. Apabila bilangan molekul menurun maka nilai TBR akan berkurang yang akan menyebabkan peningkatan jumlah pemindahan tenaga termal.

ACKNOWLEDGEMENTS

I would like to take this opportunity to express my special thanks to my supervisor, Dr. Abdul Rafeq Bin Saleman who help me a lot in completing this report by giving me suggestion, guidance and advice on writing this report. He always gives me continuous support and assistance along the way of completing this report.

Special thanks also dedicated to my beloved family, especially my father and mother for their moral support and advice during the time of completing this report. Thanks for always be there for me through thick and thin of my time. Without both of them there must be hard for me to continue this journey.

Lastly I also would like to thanks my friend who help me a lot in finalizing this report in short time period. Thanks also to everyone who had support me directly or indirectly in completing this project

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF APPENDICES

LIST OF ABBREVIATIONS

S-L	Solid-liquid
TBR	Thermal boundary resistance
FCC	Face-cantered cubic
MD	Molecular dynamic
PBC	Periodic boundary condition
r-RESPA	Revisable reference system propagator algorithm
EAM	Embedded-atom method
LJ	Lennard-Jones
UA	United atom
C	Carbon
H	Hydrogen
TJ	Temperature jump
AMM	Acoustic mismatch model
DMM	Diffusive mismatch model
DOF	Degree of freedom

LIST OF SYMBOLS

r	Position/displacement
P	Momentum
F	Force
Fs	Short range force
Fl	Long range force
t	Time
v	Velocity
a	Acceleration
E	Energy
ρ	Density
D	Dissociation energy
T	Temperature
P	Pressure
V	Volume
Å	Angstrom
H	Hamiltonian
s	Switching function
De	Well depth
R	Nuclear distance

Re	Inter nuclear distance
ve	Vibrational constant
μ	Reduced mass
m	Mass
R	Thermal boundary resistance
G	Thermal boundary conduction
k	Thermal conductivity

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Solid-liquid (S-L) interfaces which is referring to contact interfaces between solid surfaces and liquid have been found in a lot of industries such as lubrications and coatings (Liu, Wang, & Xue, 2011), thermal interface materials (Saleman et al., 2017) and electronic cooling (Yoo & Joshi, 2002). Thus, the knowledge and understanding of S-L interfaces are beneficial to control and design a number of engineering applications. The interaction between liquid with a solid also known as ‘wetting’(Park & Seo, 2011). By measuring the contact angle of the drop of liquid that being place on the surface object will help to quantify the wetting characteristic. The cohesive and adhesive force between the liquid and solid surface is well known as solid liquid (S-l) interface.(Park & Seo, 2011).

In the past the most researchers interested to look into the engineering applications in the molecular level which are not easily done experimentally. (M. Zhang et al., 2014) Such problem can be solved by using molecular dynamics simulation. Molecular dynamic simulation have been utilized to investigate a number of applications related to S-L interfaces (Hospital et al., 2015) and it is found to have less than 10% deviation with experimental results.

There are many research had been study for thermal resistance over solid-solid interface (J. Wang et al., 2020), but the study over liquid-solid interface still need to be improve in the thermal energy transfer of difference thickness of thin liquid. The thermal conductance of the interface is been recognize by the total solid heat conduction that had been go through the contact area and also the gas, in the gap (Maruyama & Kimura, 1999).

The molecular relation between solid-liquid molecule was include the interfacial thermal resistance at the S-L interface. (Wang et al., 2020)The good interfacial resistance between solid-liquid also known as Kapitza resistance.(Xue et al., 2003) The thermal resistance between solid-liquid is more high compare to solid-solid interface therefore thermal boundary resistance will play a vital role in explaining heat exchange dynamics (Milanese et al., 2016).

In previous study the researcher had revealed that the thin liquid film evaporation had no slip on the temperature wall and the Kapitza resistance was not available during the process (Zhao et al, 2011). Some of the studies stated that the interfacial thermal resistance that cross the liquid-solid interface is important during the heat dissipation (X. Wang et al., 2020). Moreover it also stated that the thermal resistance is control by the phonon density which is will cause the heat transmitted ration for two difference material (Kim, 2012). The low interface thermal resistance make it attainable to scale back heat losses and play as important role during heat transfer (Vo & Kim, 2015).

The thermal interface can be explain in two way. The first one is diffuse mismatch model (DMM) and acoustic mismatch model (AMM) (Zhang et al., 2018), which is describe by the phonon mismatch at the contacting surface. Base on molecular simulation (MD) it is explain that the thermal interface is control by the combination of interaction between solid and liquid molecules (Torii, Ohara, & Ishida, 2010) and the effect of surface structure at the interface.

Many study had been conducted related to the heat transfer at S-L interface (Maruyama & Kimura, 1999)(Xue et al., 2003)(Kim, 2012) (X. Wang et al., 2020) (Zhao et al, 2011)(Yuan, Duan, Li, Shang, & Luo, 2015)(Milanese et al., 2016)(Vo & Kim, 2015). The study about heat transfer to difference thickness of thin liquid is not been complete yet. The purpose of this project is to determine the characteristic of heat transfer over the S-L interface of simple liquid contacting crystal solid surface at difference thickness of thin liquid film. In order to obtain the result of this project, the molecular dynamic simulation had been used for the rest of this test because of the design of molecular dynamic simulation will be used to investigate the thermal resistance for both perpendicular and parallel to liquid-solid interface (X. Wang et al., 2020). Thus at the end of this project the characteristic of the thermal energy transfer at difference thickness of thin liquid can be compare.

1.2 Method of Measurement

The techniques for the TBR calculation at S-L interface that just consider phonon transport is the acoustic mismatch model (AMM) and the diffuse mismatch model (DMM) (Swartz & Pohl, 1989).

1.2.1 Acoustic Mismatch Model (AMM)

The model of acoustic mismatch (AMM) was first introduce by Khalatnikov in purpose to explain the existing of thermal energy resistance at the boundary of helium.(Peterson & Anderson, 1972) The AMM calculates the transmission coefficient depend on continuum acoustics and the mismatch in the acoustic properties of the materials forming the interface. The AMM Considers specular reflection of phonons at the interface. The AMM is better at low temperature model as the interface appears smooth and perfect. The AMM is unable to predict data at the intermediate temperature

1.2.2 Diffuse Mismatch Model (DMM)

The DMM calculates transmission coefficient based on the elastic diffuse scattering at the interface. The DMM Considers diffuse reflection at the interface. DMM is hypothetically a high-temperature model, as it is based on scattering of phonons at the interface, which is more significant at higher temperatures. The DMM is unable to predict data at the intermediate temperature.

1.3 Problem Statement

The effect of the difference thickness of thin layer film to the characteristic of heat transfer across the solid-liquid interface had been study before. However, in this test we will look at the difference of thickness for the thin layer film of 30 Å and 60 Å will impact the characteristic of the heat transfer across the solid-liquid interface. The test will be carry on by using the molecular dynamic (MD) simulation in order to compare the characteristic of the thermal energy transfer at difference thickness of thin liquid because molecular dynamic (MD) simulation will solve the equation of motion and evaluate the mathematical formula. This will help in order to study the thermodynamic properties.

1.4 Objective

The objective of this project is

1. To investigate the influence of difference liquid film thickness on the thermal energy transfer at solid-liquid interface base on thermal boundary resistance.
2. To study the influence of surface structure of (110) at solid-liquid interface base on thermal energy transfer.

1.5 Scope of Study

The scope of this study if being determine base on the objective of this project. The simulation system that will be test is a model consists of thin liquid film that is arranged sandwiched between two parallel solid walls. The solid wall is a Face-Cantered-Cubic lattice with (110) lattice structure. The liquid is consists of simple liquid of a united atom, which are liquid alkane of methane (CH_4). The simple liquid here meaning that the molecular structure of 1 carbon and 4 hydrogen will be modified to be as one atom only. However, the molecular interaction is identical to the all atom model. During the simulation proses the steady and constant amount of heat flux will be transfer across the system. The result of thermal boundary resistance (TBR) will be obtained from the test that had been conducted. The difference thickness of thin liquid film effect towards the TBR at S-L interface will also be studied. The test had been conducted several times as to make sure the repeatability is achievable and the simulation system is converged.

1.6 Significant of Study

The significant of this study is to bring benefit to all society bases on thermal energy transfer. For example, the energy transfer application at the surrounding is the bread toaster that draws electric power to heat up the filament into thermal energy that toasts the bread. Moreover, petroleum refineries apply thermal energy in several processes, cracking, reforming and treating. This processes necessarily different type of thermal energy, steam and direct heat for combustion and separation. Besides, the used of lubricant in order to reduce the thermal energy in running motor. Lastly steel and iron apply thermal energy to manufacture steel from iron ore by smelting with coke or limestone.

1.7 Flow Chart

Figure 1show the flow chart of the study

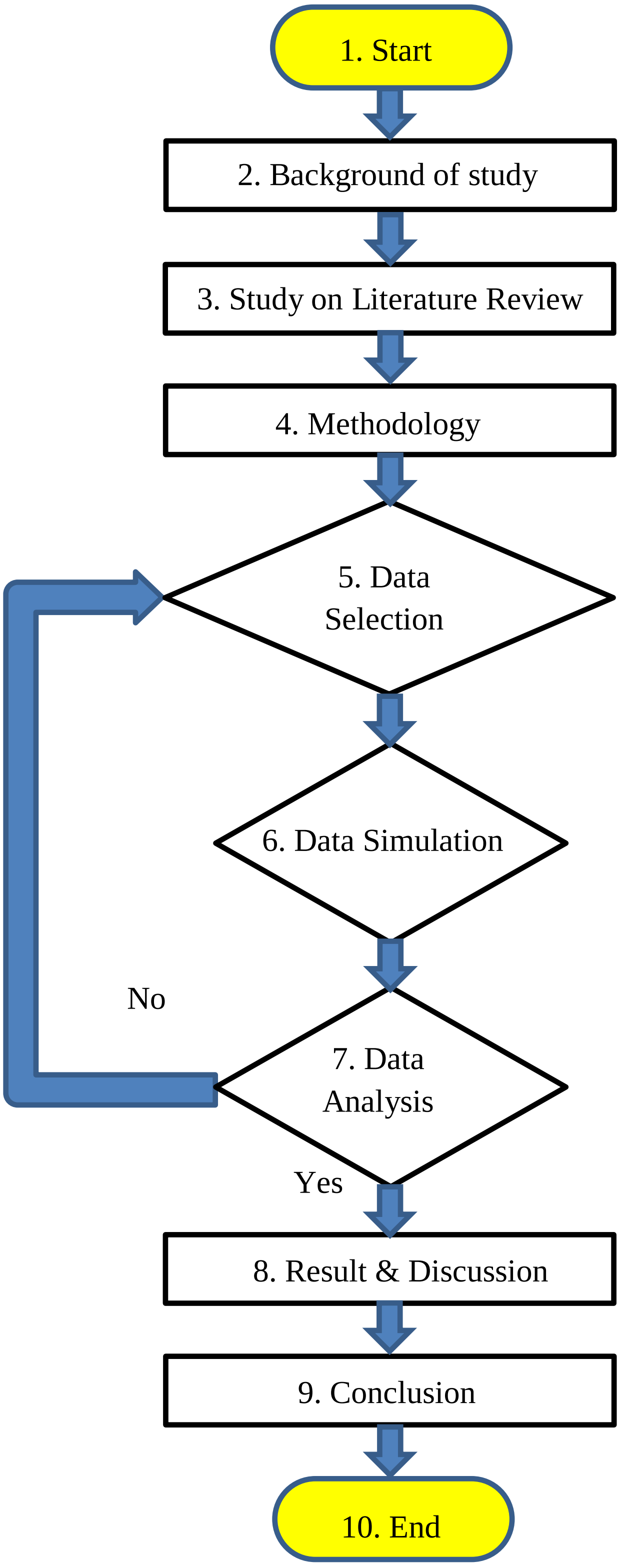

Figure 1: Flow chart of Study

Base on the figure 1, the detail of the flow chart are as follow. In Start, the title and objective of the project will be finding. The Gantt chart and the flow chat is generate after the proper discussion had been done with the supervisor. At background of study section, the finding of the journal, article and any source of material had been carried out. Base on this finding the theory and the background of the thermal energy transfer across solid-liquid interface will be written. Besides, in study on literature review, the topic of thermal energy transfer across solid-liquid interface research from the past researcher had been study to get better understanding about the topic. Literature review will be written base on this part. On methodology section, the methodology is being produce base on the difference thickness of thin liquid to get the result of thermal energy transfer characteristic. Moreover, in data selection, the parameter of this study will be selected. The parameter will be selected based on the literature review and past researcher finding. In data simulation part, the simulation will be carry out in order to get the result base on the difference thickness of thin liquid film on the thermal energy transfer. Next is data analysis section. After the result is obtained it will be analysed base on density distribution, temperature distribution, and heat flux data for the test of difference thickness thin liquid film of FCC (110) crystal plane. However if extra results obtain, the data selection will be look up again. The result and discussion will be analysed to investigate the impact of difference thickness of thin liquid to the thermal energy characteristic at solid-liquid interface. Lastly is the conclusion part. At this part, further research on thermal energy transfer at solid-liquid interface was explained. In the End, the report of this test will be written.