

**THE CHARACTERISTICS OF THERMAL ENERGY TRANSFER ACROSS SOLID-
LIQUID INTERFACES BETWEEN FACE-CENTERED CUBIC LATTICE OF 110
CRYSTAL STRUCTURE AND SIMPLE LIQUID AT DIFFERENT REDUCED
TEMPERATURE OF LIQUID**

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UNIVERSITI TEKNIKAL MALAYSIA MELAKA

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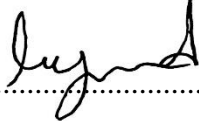
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2021

2

DECLARATION

I declare that this project report entitled “The Characteristics of Thermal Energy Transfer Across Solid-Liquid Interfaces Between Face-Centered Cubic Lattice of 110 Crystal Structure and Simple Liquid at Different Reduced Temperature of Liquid” is the result of my own work except as cited in the references.

Signature	: 
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Date	: 15 th January 2021

APPROVAL

I have checked this report and the report can now be submitted to JK-PSM to be delivered back to supervisor and to the second examiner.

Signature :.....

Name of Supervisor : Dr. Abdul Rafeq Bin Saleman

Date :.....

ABSTRACT

Solid-liquid (S-L) interfaces are phases between a solid and a liquid. It is commonly used in lubrication and coating systems where the thermal energy transport is one of the main problems for the system. Lubrication and coating systems have been studied up to molecular scale over the last few years to find the solution for thermal transport problem due to wear and friction. The characteristics of the thermal energy transport on the molecular scale are quite different from the conventional one. 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-centred cubic (FCC) lattice of 110 crystal structure and simple liquid at different reduced temperature of liquid. In this numerical study, the primary issue is the surface structure of solid and the type of liquid molecules. The characteristics of the thermal energy transfer at the S-L interfaces are evaluated based on the density, temperature jump (TJ) and thermal boundary resistance (TBR) at the interfaces. It is found that the different density, TJs and TBRs can be observed for variation of liquid reduced temperature. The findings obtained show that the reduced temperature will have a substantial effect on the characteristic of thermal energy transfer at solid-liquid interfaces.

ABSTRAK

Antara muka pepejal-cecair adalah fasa yang belaku di antara pepejal dan cecair. Bahagian ini sering digunakan dalam sistem pelinciran dan pelapisan di mana pengeluaran tenaga haba merupakan salah satu masalah utama dalam sistem tersebut. Kebelakangan ini, kedua-dua sistem ini telah dikaji sehingga ke skala molekul untuk mengatasi masalah pengeluaran tenaga haba yang disebabkan oleh kehausan dan geseran sistem. Dalam kajian yang dilakukan, ia didapati bahawa ciri ciri tenaga haba pada skala molekul adalah berbeza dengan tenaga haba konvensional. Oleh sebab itu, kajian ini telah dijalankan untuk mengkaji ciri-ciri pemindahan tenaga termal pada skala molekul di antara muka pepejal-cecair antara kisi kubik berpusat daripada 110 struktur kristal dan cecair simple pada suhu cecair yang berbeza. Masalah utama yang dihadapi dalam kajian ini adalah struktur permukaan pepejal dan jenis molekul cecair. Ciri-ciri pemindahan tenaga termal pada antara muka pepejal-cecair akan dinilai berdasarkan kepadatan cecair, lompatan suhu yang dialami dan rintangan sempadan termal pada antara muka. Melalui kajian ini, ia didapati bahawa terdapat ketumpatan, lompatan suhu dan rintangan sempadan termal yang berbeza telah diperolehi untuk suhu berkurang cecair yang berbeza. Penemuan tersebut menunjukkan bahawa suhu berkurang akan memberi kesan yang besar terhadap ciri-ciri pemindahan tenaga termal pada antara muka pepejal-cecair.

ACKNOWLEDGMENT

First of all, I would like to express my sincere gratitude to my supervisor, Dr. Abdul Rafiq bin Saleman from the Faculty of Mechanical Engineering Universiti Teknikal Malaysia Melaka (UTeM) for his continuous support, guidance and advice throughout the journey of this thesis writing. Without his grace this thesis could not become a reality. A paper is not enough for me to express the support and guidance I received from him during this study. Besides, I would like to thank to my dearest course mates especially Bong Chee Tat, Tan Jia Wei, Ain Sharmila Izzaty and Muhammad Safiuddin for giving me motivation, support and advice that eventually lifting my spirit in this thesis writing. I am extremely fortunate to have them all along for their honest feedback and assistance despite of their busy schedules. Special thanks to all my parents and family members for their moral support in completing this project. Last but not least, I am very grateful to those who had involved and contributed directly or indirectly to this project. Thank you for making this thesis writing successful.

TABLE OF CONTENTS

DECLARATION	3
APPROVAL	4
ABSTRACT	5
ABSTRAK	6
ACKNOWLEDGMENT	7
TABLE OF CONTENTS	8
LIST OF FIGURES	10
LIST OF TABLES	12
LIST OF ABBREVIATIONS	13
CHAPTER 1	14
INTRODUCTION	14
1.1 BACKGROUND	14
1.2 PROBLEM STATEMENT.....	19
1.3 OBJECTIVE.....	20
1.4 SCOPE OF PROJECT.....	21
1.5 GENERAL METHODOLOGY	22
CHAPTER 2	25
LITERATURE REVIEW	25
2.1 INTRODUCTION	25
2.2 SOLID-LIQUID INTERFACE	27
2.3 THERMAL BOUNDARY RESISTANCE.....	30
CHAPTER 3	42
METHODOLOGY	42
3.1 INTRODUCTION	42
3.2 SIMULATION DETAILS.....	43

3.3	SIMULATION METHOD	46
CHAPTER 4	49
RESULT AND DISCUSSION	49
4.1	DENSITY DISTRIBUTIONS	49
4.2	TEMPERATURE DISTRIBUTIONS	53
4.3	THERMAL BOUNDARY RESISTANCE	60
CHAPTER 5	63
CONCLUSION AND RECOMMENDATION	63
REFERENCES	64
APPENDIX	66

LIST OF FIGURES

Figure 1.5.1:	Flow Chart	23
Figure 1.5.2:	Gantt Chart	24
Figure 2.1.1:	Temperature profile of the chain	25
Figure 2.2.1:	Silica-SAMs-water model structure	27
Figure 2.2.2:	Schematic domain of the simulation domain	28
Figure 2.3.1:	Simulation system for the energy transfer through the S-L interfaces	30
Figure 2.3.2:	Simulation system for the positive heat flow direction of (110) crystal planes facing liquid CH ₄	34
Figure 2.3.3:	Surface structure of (100) crystal planes	35
Figure 2.3.4:	Surface structure of (110) crystal planes	35
Figure 2.3.5:	Surface structure of (111) crystal planes	35
Figure 2.3.6:	Definition of the slab for temperature and heat flux measurement for the positive heat flow direction of (110) crystal plane contacting CH ₄ liquid	38
Figure 2.3.7:	Density distributions of (100), (110) and (111) crystal planes	39
Figure 2.3.8:	Total heat flux average temperature jump for the two opposite heat flow direction of liquid CH ₄ contacting (100), (110), and (111) crystal planes	40
Figure 3.2.1:	Simulation system for the positive heat flow direction of (110) crystal planes facing liquid CH ₄	43
Figure 3.2.2:	Surface structure of (110) crystal planes	44
Figure 3.2.3:	Surface orientation of (110) crystal planes	44
Figure 3.2.4:	Flow orientation of (110) crystal planes	45
Figure 3.3.1:	Simulation program for 0.6T _c after equilibrated for 2 million time steps	46
Figure 3.3.2:	Simulation program for 0.6T _c after data acquisition for 20 million time steps	48
Figure 3.3.3:	Simulation program for 0.6T _c after calculating average heat flux and cumulative heat flux	48

Figure 4.1.1:	Density distributions for liquid CH ₄ contacting FCC (110) crystal planes at 0.6T _c	49
Figure 4.1.2:	Density distributions for liquid CH ₄ contacting FCC (110) crystal planes at 0.7T _c	50
Figure 4.1.3:	Density distributions for liquid CH ₄ contacting FCC (110) crystal planes at 0.8T _c	50
Figure 4.2.1:	Definition of the slab for temperature and heat flux measurement for the positive heat flow direction of (110) crystal plane contacting CH ₄ liquid	52
Figure 4.2.2:	Temperature distribution reading for 0.6T _c	54
Figure 4.2.3:	Temperature distribution graph of Liquid CH ₄ for 0.6T _c	55
Figure 4.2.4:	Temperature distribution reading for 0.7T _c	55
Figure 4.2.5:	Temperature distribution graph of Liquid CH ₄ for 0.7T _c	56
Figure 4.2.6:	Temperature distribution reading for 0.8T _c	56
Figure 4.2.7:	Temperature distribution graph of Liquid CH ₄ for 0.8T _c	57
Figure 4.3.1:	The heat flux reading for 0.6T _c after first 10 million time steps	60
Figure 4.3.2:	The graph of heat flux for 0.6T _c after first 10 million time steps	61
Figure 4.3.3:	The reading and graph of the heat flux for 0.6T _c after second 10 million time steps	61

LIST OF TABLES

Table 3.2.1:	The number of solid atoms in the x-, y- and z-axes for (110) crystal planes on one side of the simulation system	45
Table 4.2.1:	The critical temperature of liquid methane and simulation conditions of temperature	58
Table 4.2.2:	Temperature jumps for liquid methane contacting (110) crystal planes	59
Table 4.3.1:	TBR for CH ₄ liquid with 0.6T _c , 0.7T _c and 0.8T _c in x, y and z-component	62

LIST OF ABBREVIATIONS

Au	Gold
CH ₄	Liquid Methane
C ₄ H ₁₀	Butane
C ₈ H ₁₈	Octane
C ₁₆ H ₃₄	Hexadecane
FCC	Face-Centered Cubic
HBs	Hydrogen Bonds
LJ	Lennard-Jones
MDS	Molecular Dynamics Simulations
NEMD	Non-Equilibrium Molecular Dynamics Simulations
RDF	Radial Distribution Function
r-RESPA	Reversible Reference System Propagator Algorithm
SAMs	Self-Assembled Monolayers
S-L	Solid-Liquid
TBC	Thermal Boundary Conductance
TBR	Thermal Boundary Resistance

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

In the physical sciences, an interface is the boundary between two spatial regions occupied by different matter, or by matter in different physical states. The interface between matter and air, or matter and vacuum, is called a surface. In thermal equilibrium, the regions in contact are called phases, and the interface is a phase boundary. There can be several types of interfaces between same or different matter such as solid-solid interface, liquid-liquid interface, solid-gas interface, liquid-gas interface and solid-liquid interface. This study will only focus on solid-liquid interface.

The solid-liquid interface is a phase between a solid (phase α) and a liquid (phase β). The solid can be categorise into 3 types which is polar (high surface energy solid such as oxide), semi polar (intermediate surface energy solid such as cellulose acetate) or nonpolar (low surface energy solid such as hydrocarbon solid or poly-tetrafluoroethylen). The liquid can be polar (such as water alcohol) or nonpolar (such as hydrocarbon oil). The solid-liquid interfacial tension can be defined as the energy per unit area in mJm^{-1} , which depends on the nature of the solid and the liquid. For a polar solid dispersed in a polar liquid, charge separation may take place resulting in the formation of an electrical double layer (Tadros, 2014). Solid-liquid interface plays a fundamental role in a number of areas and helps to explain the

physical phenomena and structural knowledge of the interface, at the atomic scale, for example in catalysis, crystal growth, lubrication, electrochemistry, environmental science, colloidal system and in many chemical reactions. Therefore, unravelling the atomic structure at the solid-liquid interface is one of the major challenges facing by the surface science today in order to understand the physical processes in model systems (Park and Seo, 2014).

Solid-liquid interfaces have also been widely used in tribology applications that are related to lubrication and coating systems (Munir et al., 2017). Some of the example of these applications are characterisation of the thermal interface materials, production of magnetic hard disc and journal bearing design. Due to the advancement of nanotechnology in recent years, most of the lubrication and coating processes have been studied on the molecular scale. Based on the studies conducted by Tari, Nakano and Ohara (2018), it was reported that the systems that are in the molecular scale have anomalous characteristics that could not be easily determined or predicted based on the conventional macroscopic concept. Therefore, in order to address such problems, molecular dynamics (MD) simulation can be utilized as the powerful tools to reproduce the molecular-scale phenomena for the detailed analysis.

In the past, there have been a number of theoretical and experimental investigations that focus on solid-liquid interface and molecular dynamics. Molecular dynamics was first reported by Alder and Wainwright (1969) by studying a method to calculate the behaviour of several hundred interacting classical particles. The study of this many-body problem is carried out by an electronic computer which solves numerically the simultaneous equations of motion. One of the aims of the study is to compare the results with these analytical theories. Such comparisons are more clean-

cut than comparisons with experiments on natural systems because it is possible to set up artificial many-particle system with interactions which are both simple and exactly known and for which analytical theories are relatively easy to work out. Another aim of this study is to investigate the phenomena which present theories (1969) have difficulty describing because too many molecules have to be considered simultaneously.

Later, A.R.B. Saleman et al (2016) investigated the effect of the molecular length of the linear alkane in contact with each of the face-centred cubic (FCC) crystal planes on the thermal boundary resistance (TBR) at the solid-liquid interfaces. This study was conducted by using nonequilibrium molecular dynamics (NEMD) simulations where constant heat flux was applied. Different types of face-centred cubic of gold were used in this case, which are surfaces of (100), (110) and (111) crystal planes. This study investigated the effect of molecular length of the linear alkane liquids with respect to the thermal boundary resistance of the solid-liquid interfaces. It was found that on the solid wall surface of (110) crystal plane, where lattice-scale corrugation exists, molecules of liquid alkanes are adsorbed into corrugation. The thermal boundary resistance over solid-liquid interfaces were obtained based on the temperature jump at the interfaces and the heat flux, and it was found that thermal boundary resistance is influenced by the length of liquid alkane molecules, the number density of solid atoms at the surface layer and the gap distance. Therefore, it is concluded that the thermal boundary resistance is influenced by the gap distance of the S-L interfaces and the number density of solid atoms at the surface layer, which varies depending on the length of liquid alkane molecules.

Thermal rectification is a phenomenon that heat is conducted easily in one direction but much harder in the opposite direction. It was first introduced by Starr (1936). He performed experiment on the thermal energy transfer at the interfaces between cuprous oxide and copper in order to find out that there exists an asymmetrical thermal conductance. Then in the year 2002, Terraneo et al. have reintroduced the phenomenon of thermal rectification with the simulation of 1D non-linear heat conduction systems. After that, Chang et al. (2006) also reintroduced the phenomenon with the experiments of non-uniformly mass-loaded nanotubes. In 2018, a study on the thermal rectification effect at the solid-liquid interfaces was conducted by Ohara et al. Different face-centred cubic of gold with the surface of (100), (110) and (111) crystal planes contacting liquid methane (CH_4) was examined by using non-equilibrium molecular dynamics simulations. The investigation on the thermal rectification effect was performed by measuring the thermal boundary conductance (TBC) at the solid-liquid interface. The results suggest that the factors that influence the thermal rectification at the solid-liquid interface are the magnitude of the adsorption of liquid molecules and the surface structure of the solid walls that differ significantly among the three types of crystal planes.

The past studies of solid-liquid interfaces have done on many aspects such as modified surface and interaction between solid and liquid such as Ohara et al in 2016. However, the impact of the reduced temperature and the type of liquid molecules on the thermal energy transfer characteristics at the interfaces have yet to be investigated. So far in the previous studies, 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-centred cubic (FCC) lattice of 110 crystal structure 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

During pervious time, there have been a number of inquiries that focus on the thermal energy transfer characteristic at solid-liquid interface such as the influences of molecular interactions between solid and liquid (Khare, Rajesh, Pawel and Arun, 2016) and surface roughness (Priezjev and Nikolai, 2017). A number of molecular dynamics (MD) investigations on thermal boundary resistance (TBR) at the solid-liquid interfaces have been conducted which utilise simple molecules that studies the influence of the interfacial interaction on TBR at the interfaces (Barisik and Beskok, 2012) and molecular scale structure of the solid surface (Pham, Barisik and Kim, 2013). However, to this date, there is very limited substantial research on the impact of the surface structure of solid walls and the type of liquid molecules on the thermal energy transfer characteristics. Thus, this study deliberates on the effect of reduced temperature on structure quantities and thermal boundary resistance. This study investigates the characteristics of thermal energy transfer in the molecular scale at the solid-liquid interfaces between face-centred cubic (FCC) lattice of 110 crystal structure and simple liquid at different reduced temperature of liquid. Moreover, the considerations of surface structure of FCC surfaces will be described using thermal boundary resistance. Only face-centred cubic (FCC) lattice of (110) crystal structure will be used in this study.

1.3 OBJECTIVE

The objectives of this project are as follows:

1. To investigate the influence of reduced temperature on structure quantities.
2. To study the effect of reduced temperature on thermal boundary resistance.

1.4 SCOPE OF PROJECT

The scopes of this project are:

1. Only face-centred cubic (FCC) lattice of (110) crystal structure is studied in this project.
2. Only critical temperature ranges from $0.8T_C$ to $0.6T_C$ is used to analyse the performance of different factors in this project.
3. Only Reversible Reference System Propagator Algorithm (r-RESPA), one of the Algorithm methods is applied in the simulation to study the molecular dynamic in this project.
4. Only solid-liquid interface is used to calculate σ and Σ for the potential function in this project.

1.5 GENERAL METHODOLOGY

This subtopic describes the general progress for this project. The Flow Chart and Gantt Chart are shown in Figure 1.5.1 and Figure 1.5.2. There are 7 processes in flow chart which are problem statement, literature review, hypothesis, simulation, data collection and analysis, validation of data and report submission.

The general progress starts with the selection of the final year project. The title of the project has been set as “The Characteristics of Thermal Energy Transfer Across Solid-Liquid Interfaces Between Face-Centred Cubic Lattice of 110 Crystal Structure and Simple Liquid at Different Reduced Temperature of Liquid”. A total of 20 journals and articles are analysed and adopted as references in the literature review.

The method applied in the simulation for this project is Reversible Reference System Propagator Algorithm (r-RESPA). This method can be used to calculate the molecular dynamics of the lattice structure during the simulation’s analysis. This report will be submitted on 15/01/2021 prior to the due date.

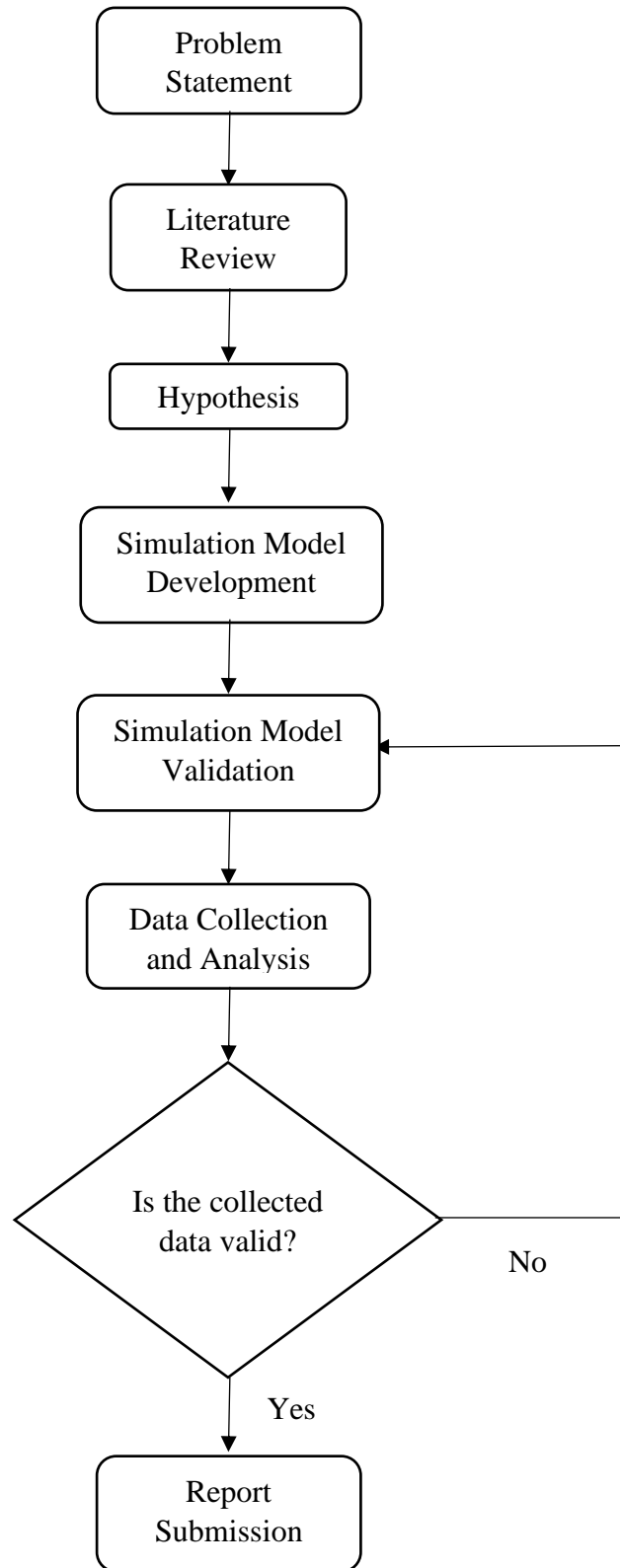


Figure 1.5.1: Flow Chart

No.	Activities	Week																								
		PSM 1														PSM 2										
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	1	2	3							
1.	Topic confirmation and discussion with supervisor	■	■																							
2.	Preparation of Chapter 1: Introduction	■	■	■																						
3.	Preparation of Chapter 2: Literature review				■	■	■																			
4.	Preparation of Chapter 3: Methodology						■	■	■																	
5.	Submission of PSM 1 Progress Report									■	■															
6.	Submission of PSM 1 Finalize Report											■	■													
7.	Preparation for PSM 1: Seminar and Presentation												■	■												
8.	Simulation and data analysis													■	■	■	■									
9.	Preparation of Chapter 4: Result and Discussion																■	■								
10.	Preparation of Chapter 5: Conclusion and Recommendations																		■	■						
11.	Preparation for PSM 2: Seminar and Presentation																				■	■				
12.	Submission of PSM 2 Finalize Report																						■	■	■	■

Figure 1.5.2: Gantt Chart