Faculty of Mechanical Engineering

THERMAL RECTIFICATION AT SOLID-LIQUID INTERFACE OF SIMPLE LIQUID IN CONTACT WITH FACE CENTERED CUBIC LATTICE

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Bachelor of Mechanical Engineering

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NIKKI HAN TIN LOON

A thesis submitted
in fulfilment of the requirements for the Degree of
Mechanical Engineering

Faculty of Mechanical Engineering

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2018

DECLARATION

I declare that this project entitled "Thermal rectification at solid-liquid interfaces of simple liquid in contact with face-centered cubic lattice" is the results of my own excepts as cited in references.

Signature : ……….……………………

Name : Nikki Han Tin Loon

Date : 16/01/2019

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 (BMCG).

Signature : ……………...............................

Supervisor Name : …………………………………

Date : …………………………………

ABSTRACT

A molecular dynamic study on the influences of the surface structure of solid on the thermal rectification at solid-liquid (S-L) interfaces of three types of face-centered cubic lattices namely are (100), (110) and (111) in contact with a simple liquid. Thermal rectification (TR) is defined as the differences in thermal energy transfer for two opposite directions of heat flow from the solid to the liquid and vice versa. In this project, the TR is evaluated based on the thermal boundary conductance TBC at the S-L of the two opposite directions of heat flow. The differences of the TBC between the two opposite directions of heat flow will be reported.

ABSTRAK

Satu kajian dinamik molekul mengenai pengaruh struktur permukaan pepejal keatas pembetulan haba pada antara muka pepejal-cecair (S-L) dengan tiga jenis kekisi berpusat muka padu kubik iaitu (100), (110) dan (111) bersentuhan dengan cecair mudah. Pembetulan termal (TR) ditakrifkan sebagai perbezaan aliran haba dari pepejal ke cecair dan sebaliknya. Dalam projek ini, TR akan dinilai berdasarkan kekonduksian sempadan termal (TBC) pada antaramuka S-L dari dua arah bertentangan aliran haba. Perbezaan TBC antara kedua-dua arah bertentangan aliran haba akan dilaporkan.

ACKNOWLEDGEMENT

First of all, I praise to almighty god for having made everything possible by giving me the strength and courage to complete this Final Year Project. I also would like to take this opportunity to express my profound gratitude and deep regards to my supervisor Dr Abdul Rafeq bin Saleman for his vital encouragement, monitoring and guidance throughout this project. Furthermore, I would like to thanks my parents, and friends for their constant encouragement without which this project would not be possible. Last but not least, I would like to express my deepest appreciation to all those who provided me the possibility to complete this project.

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LIST OF ABBRREVIATIONS

S-L	Solid-Liquid
S-S	Solid-Solid
FCC	Face Centered Cubic
TBR	Thermal Boundary Resistance
TR	Thermal Rectification
PBC	Periodic Boundary Condition
NVE	Constant Particle Number (N), Volume (V) & ∑ Energy (KE & PE)
NVT	Constant Particle Number (N), Volume (V) & Temperature (T)
NPT	Constant Particle Number (N), Pressure (P) & Temperature (T)
CPU	Center Processing Unit
AMM	Acoustic Mismatch Model
DMM	Diffuse Mismatch Model
TraPPE	Transferable Potential for Phase Equilibria
TBR	Thermal Boundary Resistance
TBC	Thermal Boundary Conductance
TRR	Thermal Rectification Ratio

LIST OF SYMBOLS

τ_p	Barostat Relaxation Time Step
$\dot{A}$	Angstrom
Φ	Interaction Energy
α	Width Control Potential
-*e*	Electron Charge
∅	Electrostatic Potential
Z	Acoustic Impedance
ρ	Density
c	Speed of Sound
$\mathbf{F}_s$	Short Range Force
$\mathbf{F}_l$	Long Range Force
E_F	Electrochemical Potential
J_S	Control Surface Heat Flux

CHAPTER I

INTRODUCTION

1.1 Background of study

Thermal rectification (TR) is a phenomenon where heat is easily flow in one direction but much harder to flow in the opposite direction between two materials. In other words, TR can also be defined as the differences in thermal energy transfer between two opposite directions of heat flow between two materials in contact with each other. The two materials in contact with each other can either be the contact between solid to solid or solid to liquid, where the contact interfaces are referred here as solid-solid (S-S) interfaces and solid-liquid (S-L) interfaces, respectively.

The phenomenon of thermal rectification was first discovered by Starr in early of 1935 during an experimental investigation of the contact between copper and cuprous oxide, where it showed thermal as well as electrical rectification. However, during that time, thermal rectification did not gets much attentions from researchers. In the year of 2002, thermal rectification was reintroduced by Terraneo et al. by utilizing a nonlinear one-dimensional chain of molecules between two thermostats at various temperatures. In the year of 2004, Li et.al conduct a similar study as the Terraneo at which Li et.al used two non-linear segments coupled together by a constant harmonic spring which use the Frenkel-Kontorova (FK) model (B.Li, 2004). In recent years, due to the development of nanotechnologies attracted considerable attention from researchers in various field to investigate thermal rectification since it can be utilized in a number of engineering applications such as thermal diode and thermal transistor (S. Pristic, 2010)

In the past, most of the investigation on the thermal rectification was done towards the S-S interfaces. As such, the studies on thermal rectification towards the S-L interfaces is less numerous. The thermal rectification at S-L interfaces as first done by Hu et al, that stated the thermal rectification of S-L interface are influence by modified the surface. Next, Murad et.al stated the thermal rectification at S-L interface relies greatly on the interfacial thermal resistance and mass density (S.Murad, 2014) (S. Murad, 2012). As for this research, the S-L interface is more priority compare to S-S as the liquid are easy to manipulate unlike solid which fix to its lattices and are hard to manipulate.

Although there are a number of studies on the thermal rectification in the past, the studies related to thermal rectification at S-L interfaces is still less numerous. As such this project would like to investigate the thermal rectification at S-L interfaces.

In the past studies of thermal rectification at S-L interfaces, the behaviour of the thermal rectification was measured based on the interfacial thermal resistance at the S-L interfaces, which is also known as Kapitza resistance, thermal boundary resistance (TBR) or thermal boundary conductance (TBC). Here, the inverse of TBR is the TBC. The interfacial thermal resistance at the S-L interfaces is defined as the measurement of resistance to the thermal energy transfer at the contacting surfaces of solid and liquid that results in temperature discontinuity at the contacting surfaces (E.T Swartz, 1989) (T. Ohara D. , 2010). Molecular dynamics (MD) simulation have revealed that the interfacial thermal resistance at the S-L interfaces was influenced by the molecular interaction between solid and liquid molecules (A. Amania, 2016) (B.H. Kim, 2008) (T.Q V. B., 2015) (M. Barisik, 2012), surface morphology (T.Q V. B., Interface thermal resistance between liquid water and various metallic surfaces, 2015) (T.Q V. B., Transport phenomena of water in molecular fludic channels, 2016) and the influences of the atomic-scale structure of solid (T. Ohara D. , 2005) (D. Toruu, 2010) (Abdul Rafeq bin Saleman).

1.2 Problem Statement

In the past, thermal rectification was investigated based on the modified surface of solid, applied external forces and influences of molecular interaction between solid and liquid. Even though in the past studies have revealed that molecular scale structure of solid surfaces influences the thermal energy transfer across solid-liquid (S-L) interfaces, the influences of molecular scale structure of solid surfaces on thermal rectification have yet to be determine. As such, this study will be focusing on the thermal rectification at the S-L interfaces between simple liquid and solid surface with the structure of face-centered cubic (FCC). The influences of the surface structure of solid surfaces on the thermal rectification will be measured based on thermal boundary conductance (TBC) at the solid-liquid interfaces. The thermal boundary conductance (TBC) at the S-L interfaces will be measure for two opposite heat flow directions across the interfaces. The thermal energy transfer across the S-L interfaces will be investigated using non-equilibrium molecular dynamics (NEMD) simulations and finally the influences of surface structure of solid on the thermal rectification will be clarify.

1.3 Objective

The aim of this research is:

I. To identify the influence of thermal rectification effects at solid-liquid (S-L) interface of a simple liquid and face-centered cubic (FCC) lattice.
II. To identify the influence of surface structure of solid on the thermal rectification at S-L interfaces.

1.4 Scope

The scopes are identified based on the objectives of this project. The simulation model which is consisted of the liquid confined between two parallel solid walls will be developed. Three type of surface structure of the face-centered cubic (FCC) lattice will be utilized, namely are (100), (110) and (111) crystal planes. In this study the simple liquid consists of a liquid with simple molecules will be utilized. A constant value and amount of heat flux with two directions of heat flows will be applied on the simulation model, one from solid to liquid and vice versa. The interfacial thermal resistance at the S-L interfaces will be evaluated by using thermal boundary conductance (TBC). The evaluation of the TBC and the related parameters needed for the evaluation will be shown later. This study will be focusing on the influences of the surface structure of the solid walls on the characteristics of TBC.

1.5 Significant of Study

The significant of this study is to identify the influences of thermal rectification at S-L interface of a simple liquid with three type of FCC by measuring the TBC at the interfaces. In addition, this study will identify the influence of surface structure of solid on the thermal rectification at S-L interfaces. The finding will clarify the characteristics of the interfacial thermal resistance at the S-L interface. The application of thermal rectification not only brings benefit to the individual but for society such as the use of lubricant in the engine to encounter the heat in the car engine and coating on the jet engine turbine to protect the blade at the high operating temperature.

1.6 Flow Chart

Figure 1.1 below show the flow chart of the final year project:

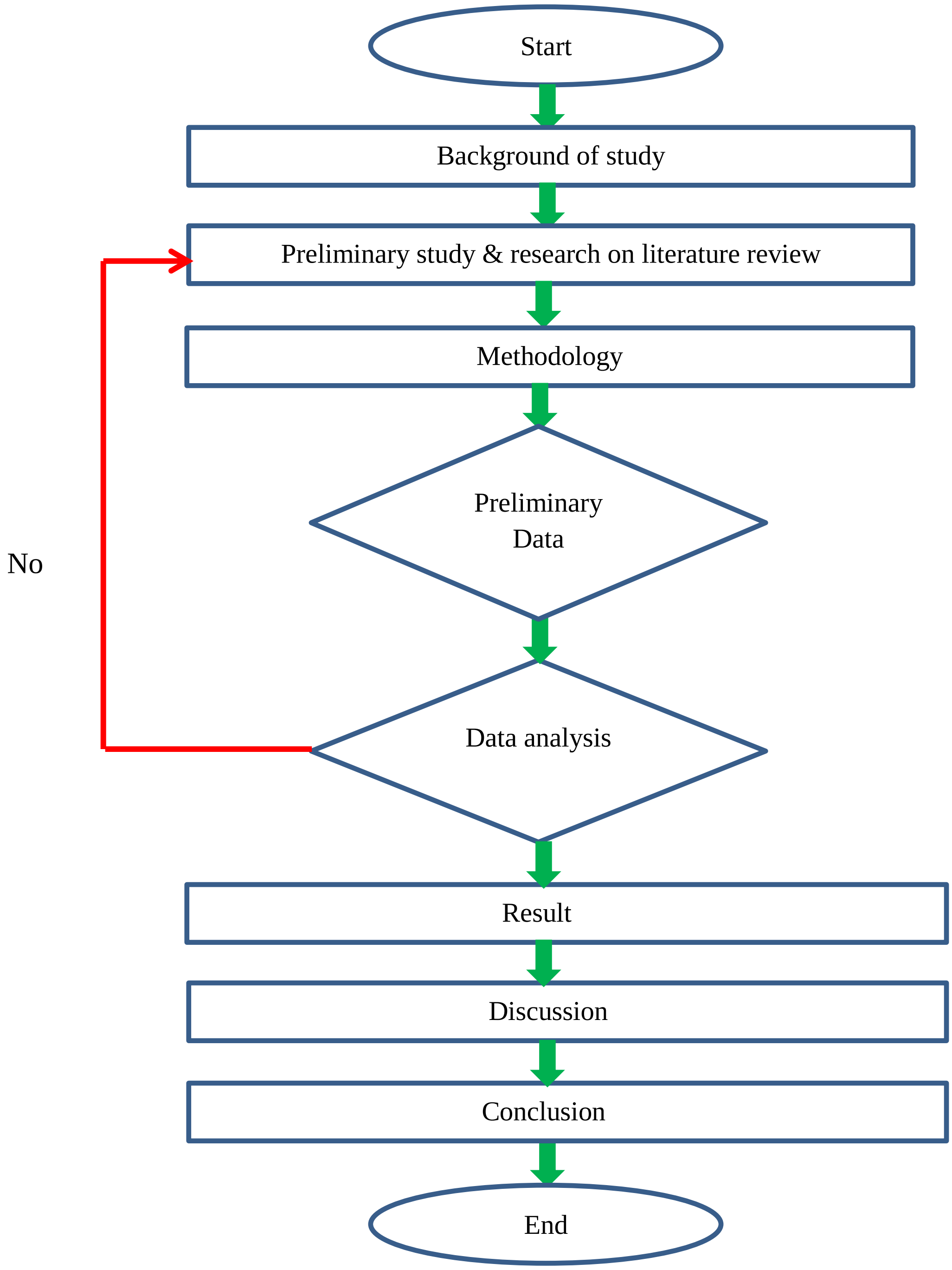

Figure 1.1 Flow chart

1.7 Flow Chart Explanation

1. Journals, article or any source of materials regarding to the project will be studied. Planning about the PSM 1 and 2 is done by constructing Gantt chart after a few discussions with lecturer.
2. The theory and research of thermal rectification at solid-solid interface and solid-liquid interface is studied for better understanding in direction and influence of heat flow.
3. After study on the previous thesis regarding about the thermal rectification of solid-liquid interface of this project. The information about the methodology of this project is obtained.
4. Verification of thermal rectification at solid-liquid interface is verified by using molecular dynamic simulation.
5. The result in this project is being analysed. The influence of thermal rectification effects at solid-liquid (S-L) interface of a simple liquid at face-centered cubic (FCC) and the influence of surface structure of solid on the thermal rectification at S-L interfaces is discussed.
6. For conclusion, a further study on thermal rectification at solid-liquid interface is described.
7. A report on this study will be written at the end of this project.

1.8 Gantt Chart

Final Year Project I (Gantt Chart)																		
No	Activity	Planning / Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	Briefing on Topic	Plan																
		Actual								M								
2	Background of Study	Plan								I								S
		Actual								D								T
3	Completed Chapter 1: Introduction	Plan																U
		Actual								S								D
4	Preliminary Study & Research on Literature Review	Plan								E								Y
		Actual								M								
5	Discuss on Literature Review	Plan								E								
		Actual								S								
6	Chapter 2: Literature Review (Draft)	Plan								T								
		Actual								E								

7	Completed Chapter 2: Literature Review	Plan								R								
		Actual																
8	Discuss on Chapter 3: Methodology	Plan																W
		Actual								B								E
9	Completed Chapter 3: Methodology	Plan								R								E
		Actual								E								K
10	Preliminary Data	Plan								A								
		Actual								K								
11	Preparation for Final Year Project (FYP I)	Plan																
	Presentation	Actual																
12	Final Year Project Presentation	Plan																
		Actual																
13	Submission Final Year Project (FYP 1) Report	Plan																
		Actual																