Available online at www.sciencedirect.com

SCIENCE DIRECT®

International Journal of Heat and Mass Transfer 49 (2006) 3401–3407

International Journal of HEAT and MASS TRANSFER

www.elsevier.com/locate/ijhmt

Molecular dynamics simulations of heat and momentum transfer at a solid–fluid interface: Relationship between thermal and velocity slip

Rajesh Khare [a,1], Pawel Keblinski [b,*], Arun Yethiraj [c]

[a] Department of Chemical and Biological Engineering, University of Wisconsin – Madison, 1415 Engineering Dr., Madison, WI 53706, USA
[b] Materials Science and Engineering Department, Rensselaer Polytechnic Institute, 110 8th St., MRC 115, Troy, NY 12180, USA
[c] Department of Chemistry, University of Wisconsin – Madison, 8305b Chemistry Bldg, 1101 University Ave., Madison, WI 53706, USA

Received 6 August 2005; received in revised form 24 February 2006
Available online 11 May 2006

Abstract

The thermal resistance of a model solid–liquid interface in the presence of laminar shear flow is investigated using molecular dynamics simulations. Two model liquids – a monoatomic liquid and a polymeric liquid composed of 20 repeat units – are confined between walls which are modeled as idealized lattice surfaces composed of atoms identical to the monomers. We find that in the absence of a velocity slip (discontinuity) at the solid–fluid interface, the mass flow does not affect the thermal interfacial resistance, but the presence of velocity slip results in an increase in the interfacial thermal resistance by about a factor of two.

Keywords: Interfacial thermal resistance; Velocity slip; Molecular dynamics

1. Introduction

A description of heat flow at the macroscopic level involves two inputs: (i) a constitutive relation between heat fluxes and driving forces, e.g., temperature gradients, and (ii) boundary conditions at the system perimeter. For example, in the absence of mass flow, one constitutive relation between the thermal energy flux, $\mathbf{j}_Q$ and the temperature gradient is Fourier's law:

$$\mathbf{j}_Q = -\lambda \nabla T, \tag{1}$$

where λ is the material bulk thermal conductivity. In the absence of internal heat sources, conservation of energy enables us to write a second order partial differential equation for the diffusive heat flow, which can be solved for the temperature profile as a function of spatial and temporal variables if appropriate boundary conditions are available. Conservation of energy requires that the thermal flux be continuous at the boundary. It is often assumed that the temperature is also continuous at the boundary.

In this work we investigate the boundary conditions for heat flow using molecular dynamics simulations. We are particularly interested in the behavior of the temperature profile at the boundary. Fluids undergoing shear flow often display velocity slip at the surface, i.e., the velocity of the fluid extrapolated to the surface position is different from the surface velocity. In an analogous fashion, it is possible for the extrapolated temperature of the fluid to be different from the surface temperature. This is the result of an interfacial thermal resistance that can have a significant effect on the thermal transport in fluids, particularly in nanofluidic systems. Computer simulations can provide molecular insight into the origin and mechanism of such interfacial thermal behavior.

Although it is often assumed that the temperature is continuous across an interface, in reality there is no

---

[*] Corresponding author. Tel.: +1 518 276 6858; fax: +1 518 276 8554.
E-mail addresses: rajesh.khare@ttu.edu (R. Khare), keblip@rpi.edu (P. Keblinski).

[1] Present address: Department of Chemical Engineering, Texas Tech University, P.O. Box 43121, Lubbock, TX 79409-3121, USA.

0017-9310/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijheatmasstransfer.2006.03.005

Nomenclature

$\mathbf{j}_Q$	thermal flux
k_B	Boltzmann constant
l_K	Kapitza length
m	mass of an atom (bead)
r	distance between two atoms
R_K	interfacial thermal resistance (Kapitza resistance)
v_x	x component of shear velocity
T	temperature

Greek symbols

δ	slip length
ε	Lennard-Jones potential energy parameter
λ	thermal conductivity
Λ	interfacial thermal conductance
ρ	density
σ	Lennard-Jones potential length parameter
τ	Lennard-Jones reduced time unit, $\tau = \sigma\sqrt{m/\varepsilon}$

firm physical basis for this assumption. In fact, Kapitza [1,2] demonstrated the possibility of a discontinuous temperature drop at an interface. This drop is quantified by the concept of interfacial conductance, Λ, which is the ratio of the heat flux (in the direction normal to interface) to the temperature drop. The inverse of Λ is the interfacial thermal resistance, also called the Kapitza resistance, R_K.

The Kapitza resistance is not significant for most solid–liquid interfaces, but can be significant in nano-structured materials. To estimate the significance of the Kapitza resistance, one can express it in terms of the "thermal resistance thickness", l_K, also called the Kapitza length, which is defined as the width of the bulk medium over which there would be the same temperature drop as that at the interface. The Kapitza length is therefore given by

$$l_K = \frac{\lambda}{\Lambda} = R_K\lambda. \tag{2}$$

Typically, in the case of a solid–liquid interface involving a wetting liquid, Kapitza length is of the order of a molecular size and thus the temperature drop at the interfaces can be neglected. However, for non-wetting liquids [3,4], l_K can be of the order of several tens of molecular sizes. In this case, the interfacial resistance might impact the thermal transport in fluids, particularly in structures involving nanoscale dimensions, such as nanofluids. Other systems where the boundary resistance plays an important role are polycrystalline high thermal conductivity materials, such as diamond [5], where grain boundaries lead to large values of l_K, despite relatively low values of R_K, because the bulk thermal conductivity is high.

The Kapitza length plays the same role in heat transfer as the slip length in momentum transfer. When a fluid is sheared by a confining surface the boundary conditions can be either stick or slip. In the latter case, the slip length, δ, describes the discontinuity of the velocity field (velocity component tangential to the solid–liquid interface) at the surface [4]. In planar shear flow geometry δ can be evaluated from

$$\delta = \Delta v_x(z=0) \Big/ \left(\frac{\mathrm{d}v_x}{\mathrm{d}z}\right)_{z=0}, \tag{3}$$

where the fluid flow direction is in the x direction, the z direction is normal to the fluid–solid interface and $\Delta v_x(z=0)$ is the velocity discontinuity at the interface. In the case of a stick boundary condition, the velocity field is continuous at the interface, and therefore $\Delta v_x(z=0)=0$ and $\delta=0$. In the case of slip, δ has a geometrical interpretation of a distance to which a linear v_x vs. z velocity profile has to be extrapolated (beyond the solid–fluid interface) to recover the same value of velocity as the solid surface velocity. For atomistically smooth solid surfaces and especially for systems showing weak interfacial bonding characteristics, both modeling and experimental studies have demonstrated a possibility of δ reaching values of several tens of molecular sizes [6–11]. The effects of non-zero values of δ become important when the characteristic fluid channel sizes are reduced to submicron or nanoscale dimensions.

The Kaptiza length can be defined in an analogous fashion in terms of the temperature drop at the interface and the temperature gradient in the liquid at the interface, i.e.,

$$l_K = \Delta T(z=0) \Big/ \left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{z=0}, \tag{4}$$

which allows one to calculate l_K without knowledge of the absolute values of the thermal conductivity or the interfacial thermal conductance.

The primary goal of this work is to elucidate the relationship between the velocity slip and thermal slip. While there have been many studies that have addressed the slip length [6–11] or the Kapitza length [1–4,12] (for systems undergoing pure thermal transport), we are not aware of any study that focuses on the possible relationship between the velocity slip and the thermal slip. To address this question, we perform a series of molecular dynamics simulations of thermal transport across solid–liquid interfaces for stationary liquids and for liquids subjected to a planar shear flow.

We report results on molecular dynamics simulations of monatomic and polymeric fluids confined between atomistically smooth surfaces, with Lennard-Jones interactions between all sites. We compare the results for the slip length and Kapitza length in three cases: (i) where the fluid is subjected to planar shear flow with the walls held at constant