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Role of surface roughness on thermal conductance at liquid–solid interfaces

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ABSTRACT

The fractal Cantor structure is introduced to characterize the surface topography of solid wall. By this fractal characterization, a molecular dynamics simulation of heat conduction in rough nanochannels is conducted to investigate how surface topography affects the thermal conductance at liquid–solid interfaces. The role of surface roughness on temperature profiles, liquid atom trajectories, interfacial interaction energy and interfacial conductance are all examined and analyzed. The results indicate that, the temperature jump at liquid–solid interfaces is observed irrespective of surface condition, and the existence of surface roughness reduces the interfacial temperature jump. When compared with smooth surface, the presence of surface roughness diminishes the motion capability of liquid atoms in the wall-neighboring region and these atoms could maintain contact with the solid surface for a long time, which intensifies the energy transfer between the liquids and solid surface and hence contribute to large thermal conductance at a liquid–solid interface. Interestingly, it is found that the thermal conductance at a rough liquid–solid interface is affected by more than just statistical roughness height, but also fractal dimension (topographical irregularity). In addition, increases in liquid–solid interaction strength, roughness height and fractal dimension are all beneficial to enhance thermal conduction at liquid–solid interfaces. In particular, a longer trapping time of liquid atoms inside the valley of the fractal surfaces is observed for a larger fractal dimension.

1. Introduction

In classical heat transfer, the assumption of interfacial temperature continuity is usually adopted in the modeling of thermal transport across the liquid–solid interface. While the performance at macroscopic scale are consistent with this assumption, recent experiments and molecular dynamics simulations which probe nanoscale thermal behaviors indicate that the temperature jump over a liquid–solid interface may be significant and the interfacial thermal conductance is greatly affected by the nature of the interface with the reduction of the system size [1,2]. In the context, understanding the interfacial thermal conductance, especially how the atomically structured solid surface plays the role, has been becoming a crucial imperative motivated by the recent development in nanocomposite materials and micro/nanofluidics [3,4].

During the past decades there has emerged a substantial body of research on the subject of thermal conductance, or equivalently its inverse, thermal resistance, at solid–solid interface [5]. For solid–solid contact, there is only a small fraction of the nominal area that is actually in contact due to the presence of surface roughness. Once the heat flux is imposed, the heat transfer through such interfaces is mainly dependent on the conduction through the contact spots. For surface in thermal contact, an imperfect junction due to the presence of surface roughness results in a sharp temperature rise across the interface. This phenomenon is called contact resistance, which is a result of the small fraction of the nominal area that is actually in contact. The main heat transfer modes through such interfaces are the conduction through the contact spots, conduction through the fluid gap, and radiation across the fluid gap. The roughness measurements show that surfaces contain roughness features at several length scales ranging from millimeter to nanometer and demonstrate self-affine property [6]. In view of the multiscale feature of rough structure, the fractal geometry has been introduced to characterize the surface topography and investigated the rough surface effects on contact resistance [7].

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Nomenclature

D	fractal dimension
e	interfacial interaction energy per unit length
F	elastic spring force,
f_x, f_y	proportional coefficient
G_k	interfacial conductance
H	nanochannel height, see Fig. 3
i	particle i
J	heat flux normal to the interface
K	wall stiffness
k_B	Boltzmann constant
L	length
m	mass
r_c	cut-off radius
r	interatomic spacing
s	number of asperities
T	temperature
u^{lj}	Lennard–Jones (LJ) potential
x, y	coordinate

Greek symbols

δ	root mean square height
ε	energy parameter of Lennard–Jones potential
η	Gaussian distributed random force
ρ	density
σ	length parameter of Lennard–Jones potential
τ	characteristic time of Lennard–Jones potential
Γ	friction constant

Subscripts

l	liquid
low	low wall
s	solid

Superscript

$*$	reduced unit

Differing from contact resistance, the Kapitza resistance (also known as interfacial thermal resistance or thermal boundary resistance) exists even at atomically perfect interfaces. In other words, the Kapitza resistance exists no matter whether the surface is rough or not. The phenomenon of Kapitza resistance is that, due to the differences in electronic and vibrational properties in different materials, when an energy carrier (phonon or electron) attempts to traverse the interface, it will scatter at the interface. Owing to relatively good contact between the liquids and solid surface, the Kapitza resistance at the liquid–solid interface is rather small and usually considered negligible when compared with contact resistance (particularly those including gas gaps) [2,8]. Therefore, very few studies have focused on the surface effect on thermal conductance at liquid–solid interface in macroscale systems.

In nanoscale systems, the thermal resistance due to molecular level ordering at liquid–solid interface is evident even for the perfect smooth surface. In other words, the Kapitza resistance, which is negligible in macroscale, may be significant due to the fact that the thermal resistance monotonically increase with the reduction of the system size. Considering that the experimental approaches are difficult to measure the interfacial thermal conductance at the nanoscale, the molecular dynamics simulation has been the primary way to probe the microscopic thermal behavior at the liquid–solid interface [8–12]. Several attempts have been performed to study the interfacial thermal conductance with particular attention paid to the influence of liquid–solid interaction, wettability, surface roughness and confined scale [2,13–15]. Wang and Keblinski [2] investigated the role of wetting and regular nanoscale roughness on thermal conductance at liquid–solid interfaces. However, how the detailed nature of surface topography, including the statistical roughness height and fractal dimension (i.e. topographical spectrum), affect the thermal conductance at the liquid–solid interface is still not well investigated.

Therefore, we herein report a molecular dynamics simulation on the thermal conductance for liquids confined in nanochannel incorporating surface topography as characterized by fractal geometry. The effects of surface roughness on temperature distribution (especially the interfacial temperature jump) and motion behavior of liquid atoms are presented and compared with corresponding smooth interface. In addition, the roles of liquid–solid interaction strength and surface topography (including the roughness height and fractal dimension) on the interfacial interaction energy and thermal conductance are all investigated and discussed.

2. Fractal representation of surface roughness

It is well documented that the surface roughness at all magnifications appears quite qualitatively similar in structure and demonstrates the multiscale property [6,16–20]. The roughness profiles nearly always follow power laws and hence create a self-affine property. The fractal representation, which utilizes the self-affine fractal dimension to indicate the topography spectrum, is suggested to give a more realistic characterization of rough surfaces. In the current study, the Cantor fractal is introduced to characterize the multiscale and self-affine nature of rough surfaces. The fractal Cantor structure, which is developed by Borodich and Mosolov [21], and modified by Warren et al. [6], can be achieved by joining the segments at successive stages of the Cantor set. As shown in Fig. 1, the horizontal length and salient height of the $(n+1)$th level of the Cantor set surface profiles are

$$L_{n+1} = \left(\frac{1}{f_x}\right) L_n = \left(\frac{1}{f_x}\right)^{n+1} L_0 \tag{1}$$

$$h_{n+1} = \left(\frac{1}{f_y}\right) h_n = \left(\frac{1}{f_y}\right)^{n+1} h_0 \tag{2}$$

where f_x, f_y are the proportional coefficient, in which $h_0 = 2\delta$ (δ is the root mean square height) [6].

For a Cantor set surface, its self-affine fractal dimension can be calculated by [6]

$$D = 1 - \frac{\ln f_y}{\ln s f_x} + \frac{\ln s}{\ln s f_x} \quad (1 < D < 2) \tag{3}$$

where s corresponds to the number of asperities on a repeating segment. The previous investigations have indicated that, once the fractal dimension, D, and statistical roughness height, δ, are obtained from a real rough surface, then the parameters f_x, f_y and s can be determined, and finally the quantitative characterization

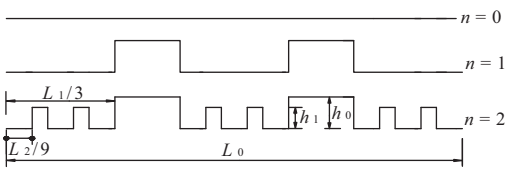

Fig. 1. Generation of fractal Cantor structure ($s = 3$).