International Communications in Heat and Mass Transfer 98 (2018) 85–95

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Molecular dynamic study on crossover of equilibrium time of conduction for silicon/silicon and silicon/silicon carbide pairs on nanoscale

Xianhua Nie, Li Zhao*, Shuai Deng, Yue Zhang

Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), MOE, Tianjin University, Tianjin 300350, China

ARTICLE INFO

Keywords:
Crossover
Phonon heat conduction
Molecular dynamics simulation
Processors

ABSTRACT

Crossover of equilibrium time during conduction was discovered using molecular dynamics (MD) simulation. In this letter, two material-pair systems, Si/Si pair and Si/SiC pair, were simulated at different temperatures and temperature differences. The temperature of Si inside Si/SiC pair was set at 280.00 K, and temperatures of SiC were set as a certain absolute value based on temperature difference settings. In addition, results from Si/Si pair were also applied as reference groups. Moreover, size effects on the crossover were also evaluated. The results suggest that there are reverse temperature differences existing where the crossover of equilibrium time of Si/Si and Si/SiC occurs. When the initial average temperature of the two material-pair is higher than 280.00 K, the equilibrium time of Si/SiC pair is higher than that of Si/Si pair initially and as the temperature difference between materials increases to 55.33 K, the equilibrium time of Si/Si pair becomes higher than that of Si/SiC pair. Similar conclusion can be obtained when the initial average temperature is lower than 280.00 K, and the reverse temperature difference is 94.98 K correspondingly. The discovery of the crossover and reverse temperature difference in this work would be beneficial to studies on heat transfer enhancement for processors.

1. Introduction

1.1. Background

Nowadays, computer and supercomputing technology are widely applied in various fields. As a core component (as shown in the red frame of Fig. 1), processor is integrated with more and more transistors in order to deal with much more complex tasks and meet requirements of a much higher computational speed. According to Moore's law, the number of transistors integrated in processors would be doubled about every 18–24 months, and their performance would be doubled simultaneously. However, highly integrated processors also lead to the power increase, and it results in a rapid increase in temperature of processors [1]. Consequently, if the heat is no dealt with properly, the stability of processors would be reduced significantly [2,3]. Yeo et al. [4] indicated that the temperature increased by 10–15 °C, life expectancy would reduce by half. Moreover, this limits the further development of high performance processors.

Therefore, thermal management becomes a challenge, and both active design (e.g. thermoelectric cooling [5] and microchannel [6]) and passive design (e.g. natural convection driven by temperature difference), as shown in the blue frame of Fig. 1, have been proposed. However, in these studies, processors are always cooled by additional equipment such as micro channels, fans and thermoelectric coolers, and this can result in an increase in the complexity of construction, high maintenance costs and limited life. Therefore, new approaches of thermal management of processors should be further explored.

1.2. Literature review of studies on Si and SiC

Furthermore, researches on thermal management of processors from material aspect, can be considered as a new starting point. Specifically, both Si and SiC are proven to be promising materials applied to produce high performance processors [7,8]. Only by understanding the heat conduction of processors on nanoscale, can the problem of thermal management be fundamentally resolved. However, different from macro Fourier conduction, sizes of transistors integrated in processors are always in nano-level. Qiu et al. [9] carefully reviewed thermal transport properties on nanoscale over the past two decades. Jean et al. [10] studied thermal conductivity of nano Si materials from the phonon point of view. Moreover, considering diffusive and ballistic limits respectively, Liu et al. [11] modelled phonon transport in Si materials based on thermoelectric technology. Besides the steady state studies, Shomali et al. [12] studied transient heat conductions of 3-D nano transistors, and filled gaps existing in transient 3-D conduction modeling for nano transistors.

---

* Corresponding author.
E-mail address: jons@tju.edu.cn (L. Zhao).

https://doi.org/10.1016/j.icheatmasstransfer.2018.08.015

Nomenclature

c_p	heat capacity
k_B	Boltzmann constant
N	the number of atoms
N_f	the number of degrees of freedom
m	mass of atom
Q	heat transfer rate, W
T	temperature, K
v	velocity of atoms
$V^{Tersoff}$	bond energy of atoms system

Greek symbols

τ	equilibrium time, ps
ω	vibrational frequency, THz

Abbreviations

MD	molecular dynamics
NVE	micro-canonical ensemble
NVT	canonical ensemble
Si	silicon
SiC	silicon carbide
VACF	velocity autocorrelation function
VDOS	vibrational density of state

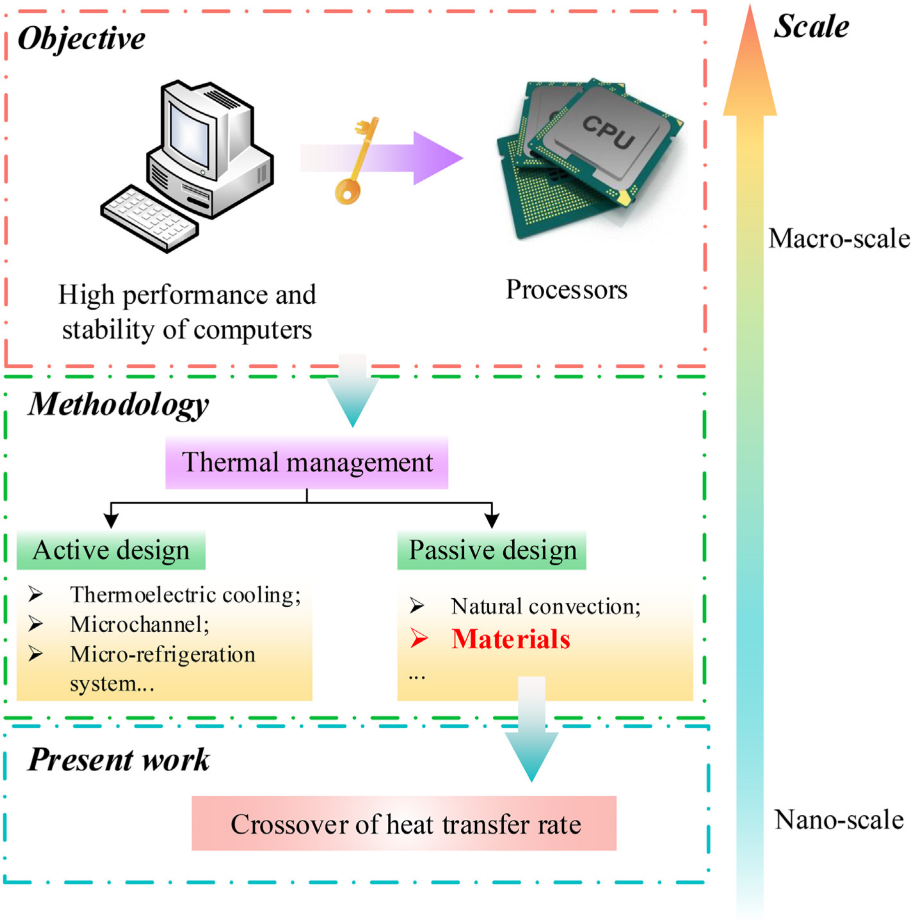

Fig. 1. Recent advance of researches on thermal management of processors.

Furthermore, considering the wave nature of phonon, Li and Ye [13] considered effects of scattering and interference on phonon transport between different materials. In addition, Luckyanova et al. [14] showed the existence of coherent phonons in superlattices (SLs). Furthermore, Ravichandran et al. [15] studied the crossover from incoherent to coherent phonon in SLs, and the interface density was selected as an important factor. Their results provided new understandings on phonon transport between different materials. Based on which, some new factors affecting heat conduction through SLs such as the roughness of the interface [16,17] and structures of cells [18], were also studied.

1.3. Present study

However, few studies focused on processors' conduction enhancement from the materials point of view. According to recent researches [13–15], compared to phonon transport between same materials, energy dissipation of phonons would be larger when phonon transfer between different materials. Thus, there naturally emerges a question: how about heat conduction characteristics on the scale of phonon when considering the effect of consistence of materials? Concretely, whether this effect would result in a completely different phenomenon on the phonon scale contrast to conventional knowledge or not should be further studied. Although a literature research on researches of such