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A molecular dynamics study of interfacial thermal transport in heterogeneous systems

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Abstract

Non-equilibrium molecular dynamics software was developed to study thermal transport at the nanoscale. Lennard–Jones parameters of pure argon (mass and bond strength) were systematically modified to create heterogeneous thin film systems, including layered systems and nanocomposites, to investigate the influence of interfaces on thermal conductivity. Results were analyzed using combinations of kinetic theory and a thermal resistance network model together with the acoustic mismatch model (AMM). The introduction of a second material into an argon film generally decreased its overall thermal conductivity. Moreover, the presence of a nanoparticle was less influential in reducing thermal conductivity than the addition of a thin layer.

Keywords: Molecular dynamics; Interfacial thermal resistance; Nanoparticle

1. Introduction

The ever-increasing demand for faster integrated circuits, larger data storage capacity, and better medical diagnostic and treatment capabilities has jumpstarted the field of nanoscience. Moreover, modern silicon microelectronics are now firmly in the nanoscale regime (<100 nm). As devices approach the nanoscale, many standard tools for solving engineering problems reach a limit of applicability because of failures in the assumptions from which those tools are built. Thermal management is one of the most frequently encountered problems at this design level, yet processes such as refrigeration, cooling and power generation would benefit largely from advances in thermal efficiency and thermal management. However, a complete picture illustrating the mechanisms that influence nanoscale thermal transport has not yet taken form. Heat flow can be inhibited or enhanced by a number of phenomena including but not limited to interstitial atoms, vacancies, pores, single atom or multi-atom (nanoparticles) impurities, lattice strain, interfaces, edge and screw dislocations, and grain boundaries. The extent to which each of these phenomena plays a role in influencing thermal transport is relatively unknown, thus an analysis of these mechanisms is necessary in order to develop a better understanding of nanoscale heat transfer. In particular, interfacial effects are an example of a mechanism which can be critical at small length scales, and through thorough investigation, its role in the larger picture of nanoscale thermal transport can be made clearer [1].

Previous research has shown that molecular dynamics (MD) is a viable method for providing insight into the nanoscale world, especially where thermal transport is concerned [2–8]. Depending on the size and state of the system, as well as how well the underlying physics are understood, MD can provide the necessary properties, such as thermal conductivity, for use in already existing tools and techniques, or slightly modified ones. More importantly, MD is adjustable and can uncover trends that can lead to a

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Nomenclature

Latin characters

a_0	equilibrium lattice constant
C	heat capacity
g	spring constant of harmonic oscillator
$\hbar$	Planck's constant divided by 2π
k	thermal conductivity
k_B	Boltzmann's constant
$\mathbf{k}$	wavevector
k_{eff}	effective thermal conductivity
ℓ	phonon mean free path (MFP)
m	atomic mass
Q	heat flux
r_c	atomic interaction cut off distance
r_{ij}	separation distance between atoms i and j
r_0	equilibrium separation distance
R_B	interfacial/thermal boundary resistance
T	temperature
x	horizontal simulation cell dimension (width)
y	lateral simulation cell dimension (height)
Z	lateral simulation cell dimension (depth)
Z_i	acoustic impedance of material i

Greek symbols

$\alpha_{i\to j}$	transmission probability of phonons traveling from material i to material j
$\Gamma_{i,j}$	AMM transmission coefficient of material i and mode of propagation j
ΔT	temperature difference
ε	Lennard–Jones well depth parameter
θ	angle of incidence of phonon on interface
Θ_D	Debye temperature
v_i	mean phonon speed of sound of material i
v_s	speed of sound
ρ_i	density of material i
σ	Lennard–Jones length scale parameter
τ	mean time between phonon collisions
Φ_{LJ}	Lennard–Jones potential
ω_D	Debye frequency

better overall understanding of the underlying physics present in special materials. For instance, Lukes et al. [4] investigated nanoporous thin films using non-equilibrium molecular dynamics (NEMD). They found that as the film's porosity increased, the dependence of thermal conductivity on temperature decreased. Moreover, the thermal conductivity became independent of temperature for pores of 5 or more atomic vacancies. Volz et al. [9] investigated the interfacial effects in silicon–germanium superlattices and discovered that strain greatly affects the overall thermal conductivity of the superlattices, all the while showing an improved agreement with experimental values. Abramson et al. [5] used NEMD simulations to study how various factors affect the thermal conductivity of bi-material thin films containing one or more solid–solid interfaces. Results suggested that variation of material composition ratios had little influence on the thermal behavior observed at or near the interfaces and that the inclusion of multiple interfaces within a bi-material film did not produce a proportional decrease in its overall thermal conductivity. In addition, a significant decrease in thermal conductivity due to lattice strain was observed when a coherent interface between two materials of different lattice constants was forced. Stevens et al. [10] utilized NEMD to study the thermal boundary resistance between two FCC structured Lennard–Jones crystals well above the Debye temperature. The study showed a strong temperature dependence of thermal boundary resistance R_B, suggesting that inelastic scattering of phonons at the interface plays a major role in thermal transport.

The most important factor determining the success of a classical MD simulator is its interatomic potential. The Lennard–Jones interatomic potential, also known as the LJ, 12–6, or 6–12 potential, is the best known and the one most commonly used for studying thermal transport. It provides a fairly realistic description of the interaction between two electrically non-conductive elements with filled valence shells. For a pair of atoms i and j the Lennard–Jones potential is:

$$\Phi_{LJ}(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

where r_{ij} is the separation distance between two atoms. The well depth parameter ε defines the strength of interaction between two like atoms at their lowest possible energy state, which corresponds to a separation distance equal to the nearest neighbor distance r_0. The separation parameter σ defines a length scale over which the interaction occurs; it is the distance between two atoms where their relative energy potential is zero. In a heterogeneous Lennard–Jones system with one or more interfaces, interfacial thermal resistance is influenced by the relative values of mass and the Lennard–Jones parameters. This is expected since the interatomic potential plays a large role in determining the thermal conductivity. To illustrate the effect on interatomic potential, Fig. 1 compares the original Lennard–Jones potential for argon to two ε-modified potentials. As ε increases, the well depth increases, effectively making it more difficult for the atoms to travel away from their equilibrium positions. Conversely, as ε decreases, the well depth decreases and the atoms feel less restricted in motion. Since phonons are influenced by atomic motion, it is evident that thermal transport will consequently be affected. It is the intention of this paper to study how variables such as mass and interatomic potential affect interfacial thermal resis-