



Tunable thermal rectification in silicon-functionalized graphene nanoribbons by molecular dynamics simulation



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ABSTRACT

In this paper, we investigate thermal rectification in hybrid pristine and silicon-functionalized graphene nanoribbons (GNRs) using nonequilibrium molecular dynamics simulations. The heat flux is larger from the functionalized section to the pristine section than that in the opposite direction. It is found that thermal rectification can be tuned through the Si/C ratio and silicon distribution. A moderate Si/C ratio and patterned arrangement are preferable to obtain a higher rectification factor. The rectification factor is also sensitive to the temperature difference and the mean temperature. As the length of the system increases, the rectification factor decreases gradually due to the emerging of diffusive effect in nanoscale GNRs. Furthermore, we calculate the vibrational density of states to explain the underlying mechanism of thermal rectification.

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1. Introduction

Thermal management is becoming more and more important in electronics industry due to the continuously shrinking feature size of devices and the increase in clock speed. Similar to electronic diodes, the thermal rectifier has useful applications not only in phononic devices and thermal logic [1] but also in energy harvesting materials and information processing [2]. With a better understanding of physical mechanisms causing thermal rectification, heat dissipation and transport in nanoscale could be well manipulated. Thermal rectification is a phenomenon where the magnitude of heat flux in one direction is larger than that in the opposite direction [3–5]. In practice, the nanostructured thermal rectifier has been achieved in multi-wall carbon or boron nitride nanotubes that were unevenly mass-loaded with a much heavier molecular species, C₉H₁₆Pt [3]. Inspired by the realization of thermal rectification in experiment and progress in fabrication technology, research on thermal rectifier has become a hot topic of nanoscale thermal transport.

Graphene, a two dimensional single layer of carbon atoms arranged in a honeycomb lattice, has been the focus of extensive studies ever since its experimental isolation in 2004 [6] because of

a number of fascinating properties it exhibits, including extraordinary high carrier mobility [7,8] and mechanical strength [9]. In addition, the thermal properties of graphene are also of fundamental and practical significance in nanoscale thermal management owing to experimentally observed superior thermal conductivity [10–12]. In recent years, many theoretical studies on thermal rectification have been conducted in graphene based systems through molecular dynamics (MD) simulations [13–20]. Yang et al. [13] demonstrated excellent thermal rectification efficiency in trapezia shaped and two rectangular graphene nanoribbons (GNRs) with different width. They found that the heat flux runs preferentially along the direction of decreasing width. Hu et al. [14] investigated the thermal conductivity of the asymmetric GNRs of triangular shapes and found significant thermal rectification. Their results showed that the thermal conductivity from the narrow to the wider end of such a triangular GNRs was less than that from the wider to the narrow end and the triangular GNRs with vertex angle of 30° and armchair bottom edge was found to have the largest thermal rectification. Pei et al. [15] reported thermal rectification in the interface of carbon isotope doped graphene and found that tensile strain leads to an increase in the interfacial thermal resistance and thermal rectification. Wang et al. [16] studied the thermal rectification effect in asymmetrically defected GNRs and the effects of design parameters. The optimum conditions for thermal rectification were recommended in their work. Their simulations indicate that spatial asymmetry in geometry is a key factor to

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Nomenclature

d	thickness, nm
E	overlapped phonon energy of vibrational density of states, eV
h	Planck constant, eV s
J	heat flow, W
k_B	Boltzmann constant, J/K
l	effective phonon mean free path, nm
L	system length, nm
m	atomic mass, kg
N	number of atoms
T_0	average temperature, K
T_L	temperature of the heat bath in the left, K
T_R	temperature of the heat bath in the right, K
w	width, nm
κ	thermal conductivity, W/m K
κ_∞	thermal conductivity of infinitely long graphene nanoribbons, W/m K
ν	frequency, Hz
v	velocity, m/s

realize thermal rectification. Other proposed thermal rectifiers in graphene show that the thermal rectification can also be tuned greatly through inhomogeneous external perturbation [17] and strain engineering [18]. Therefore, graphene is a good candidate as a thermal rectifier.

However, the mechanism leading to thermal rectification is still under debate. Many researchers adopt match/mismatch of the phonon spectra between the two sides of a rectifier to explain the asymmetric thermal rectification [16,17,21,22]. There is larger overlap of the phonon spectra in the direction of high heat flux and big mismatch of the phonon spectra in the reverse direction. But Wang et al. [23] found that the direct relation between overlap or separation of the vibrational density of states and the thermal rectification is not obvious in the investigation of bi-layer nanofilm. Actually, many factors are responsible for the thermal rectification depending on materials, geometry and surface roughness, etc.

Recently, chemical functionalization of graphene by introducing atoms and atomic groups has attracted as significant attention as a way to modify its thermal properties [24,25]. Previous studies have found that the thermal conductivity of hydrogenated and fluorinated graphene is reduced, where the magnitude of reduction greatly depends on the distribution and coverage of hydrogen or fluorine atoms [26,27], suggesting that functionalization could serve as an effective way to modulate the thermal conductivity of graphene and be useful in the thermal management of graphene-based nanoelectronic devices. Moreover, composites of Si nanoparticles well dispersed in the graphene sheets have been demonstrated to improve Li ion storage capacities and cycling stability as battery anodes [28,29]. This Si–graphene composite electrode achieved an unprecedented reversible capacity of around 1100 mAh g⁻¹ at 8 A g⁻¹. In consideration of advantages of such Si–graphene nanocomposites as electrode materials, they will play an important role in advanced wearable electronics and the storage of renewable energy.

Thermal rectification in hybrid graphene–graphene has also been investigated where in the Kapitza thermal resistances play important roles [30]. However, in contrast to the comprehensive study on thermal rectification of graphene-based systems, thermal rectification of chemically functionalized graphene has not been

well studied and whether thermal rectification can be affected by the arrangement of absorbed atoms is still not clear.

In this letter, we investigate thermal rectification in silicon-functionalized graphene using classical nonequilibrium molecular dynamics (NEMD) method. We find the silicon-functionalized graphene demonstrates significant thermal rectification and the rectification factor can be strongly affected by the distribution and coverage of silicon atoms. We further investigate the effect of temperature difference, mean temperature and system length on thermal rectification.

2. Model and simulation setup

The schematic of asymmetric GNRs configuration is shown in Fig. 1. Half of the GNRs is patterned functionalized by silicon atoms which are arranged in regular strips parallel to the heat flux. In order to compare the silicon distribution dependence of thermal rectification, the GNRs with randomly distributed silicon atoms is also studied. The Si/C ratio is defined as the ratio of the number of silicon atoms to the total number of carbon atoms in the right side of the GNRs. The armchair and zigzag edges of the GNRs are orientated along the length and width direction, respectively. The sample is around 20 nm long and 5 nm wide. The periodic boundary condition is applied to the width direction to eliminate the edge effects. The outmost columns of atoms at the two ends of the GNRs in the length direction are fixed to avoid the sublimation of atoms, and a free boundary condition is applied to the cross-plane direction.

All MD simulations are performed using LAMMPS [31] package with a time step of 0.5 fs throughout. A reactive empirical bond order (REBO) potential [32] is considered to describe the C–C bonding interaction because of its accuracy in describing bond strength and anharmonicity of carbon materials. In the REBO potential, the total potential energy of the system can be written as

$$E_b = \sum_i \sum_{j(>i)} [V_R(r_{ij}) - b_{ij}V_A(r_{ij})] \quad (1)$$

where E_b is the total chemical binding energy, r_{ij} is the distance between pairs of nearest neighbour atoms i and j , b_{ij} is a many-bond empirical bond order between atoms i and j . $V_R(r)$ and $V_A(r)$ are the repulsive and attractive pairwise interactions, respectively.

$$V_R(r) = f_c(r)(1 + Q/r)Ae^{-\alpha r} \quad (2)$$

$$V_A(r) = f_c(r) \sum_{n=1,3} B_n e^{-\beta_n r} \quad (3)$$

where the interaction parameters Q , A , α , B , β are used to fit the pairs terms, the detailed parameters are given in Ref. [32]. The function $f_c(r)$ is the truncation function that limits the range of the covalent interactions, and is expressed by

$$f_c(r) = \begin{cases} 1 & r < D_{\min} \\ [1 + \cos((r - D_{\min})/(D_{\max} - D_{\min}))]/2 & D_{\min} < r < D_{\max} \\ 0 & r > D_{\max} \end{cases} \quad (4)$$

where D_{\max} and D_{\min} define the distance over which the function goes from one to zero. The C–Si and Si–Si interactions are modeled with the Tersoff potential [33,34].

In the NEMD simulation, silicon atoms are placed 2.0 Å above the graphene surface which are within the cutoff radius of C–Si bond of Tersoff potential. Before starting the simulation, the atomic structure has been fully optimized in a microcanonical ensemble by

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