

Phonon Transport of Zigzag/Armchair Graphene Superlattice Nanoribbons

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Abstract

Nanostructured thermoelectric materials are promising for modulating physical properties to achieve high thermoelectric performance. In this paper, thermal transport properties of armchair/zigzag graphene superlattice nanoribbons (A/Z graphene SLNRs) are investigated by performing nonequilibrium molecular dynamics simulations. The target of the research is to realize low thermal conductivity by introducing single-vacancy point defects. Our simulations demonstrate that the thermal conductivity of A/Z graphene SLNRs depends nonmonotonically on periodic length. In addition, introducing single-vacancy point defects into the superlattice nanoribbons could decrease the phonon tunneling in superlattice nanoribbons, so that the thermal conductivity could be reduced further. Furthermore, a monotonic dependence of the thermal conductivity of A/Z graphene SLNRs with length of zigzag part in periodic length is discovered. This phenomenon is explained by performing phonon property analysis. Our simulations deliver a detailed phonon transport in A/Z graphene SLNRs and provide useful guidance on how to engineer the thermal transport properties of A/Z graphene SLNRs for applications of nanoribbon-related devices in thermoelectrics.

Keywords Graphene superlattice nanoribbon · Molecular dynamics simulation · Phonon transport · Single-vacancy point defect

1 Introduction

Graphene, a two-dimensional (2D) single layer of graphite, has gained much attention because of its excellent properties such as exceptional mechanical strength [1, 2], supe-

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rior high thermal conductivity [3-5], and intrinsic electron mobility [6-8], making it a promising super-material for nanoelectronics [9, 10]. The significantly high charge carrier mobility of graphene is due to the unique energy band structure of the itinerant pi-electrons near the Fermi energy that can be described as massless Dirac fermions. Besides, the exceptional mechanical strength and extremely high thermal conductivity are primarily due to the sp2-hybridized bonding of carbon atoms in graphene with hexagonal honeycomb lattice. It has been reported that thermal conductivity of graphene exfoliated mechanically is about 5000 W·mK⁻¹, which is extremely high [11]. However, it is found by experiment that the thermal conductivity of suspended graphene with defects varies between 1800 W·mK⁻¹ and 400 W·mK⁻¹ because the introduced defects result in extra phonon scattering [12]. In addition, it is revealed that the quasi-ballistic conduction of electrons could be preserved by the defects near the boundary. The recent investigations show that the electronic properties of carbon nanotube thin films were enhanced by defect modulation [13]. Inspired by those studies, researchers discovered that the thermal and electronic transport properties of graphene could also be modulated by controlling the bonding configuration and direction of the embedded defect in graphene [14].

The performance of thermoelectric devices is usually characterized by the figure of merit, expressed as $ZT = S^2 \sigma T / \kappa$, where S, σ , T, and κ are the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity of the material, respectively. Higher figure of merit indicates larger efficiency of energy conversion in the thermoelectric devices. To realize efficient thermoelectric devices, reducing thermal conductivity of nanostructured materials is a necessary step [15-17]. Introducing interfaces in thermoelectric materials can tune phonon transport, which plays an important role in solving this challenge. Si/Ge core/shell nanowires [18–20] and Si/Ge superlattice nanowires [21-23] attract great attention and are reported to have very low thermal conductivities because of the strong interfacial phonon scattering and thus the ZT coefficient can be improved. However, researchers have demonstrated that interface modulation and coherent phonons are two competing mechanisms controlling the heat conduction in Si/Ge superlattice nanowires [23]. When periodic length is extremely small, the coherent phonons emerge in Si/Ge superlattice nanowire and thermal conductivity cannot be reduced further, which is a barrier to maximize ZTvalues of superlattice nanowires used for a high-performance thermoelectric material.

To balance the competing nature of small thermal conductivity and large electrical conductivity, we intuitively construct a superlattice composed of armchair and zigzag graphene. The interface between armchair and zigzag graphene nanoribbons may significantly affect the thermal conductions of the superlattice. In addition, defects can be introduced into graphene and expected to prevent the coherent phonons in superlattice nanoribbons, thus the thermal conductivity is reduced further. In this paper, we construct a series of armchair/zigzag graphene superlattice nanoribbons (A/Z graphene SLNRs) and study the phonon transport in superlattice nanoribbons using nonequilibrium molecular dynamics (NEMD) simulations. The effects of geometry and single-vacancy point defects on thermal conductivity are explicitly considered.



Fig. 1 Schematic of a typical A/Z graphene SLNR used in the MD simulations. Color code: gray: C, pink: H (Color figure online)

2 Model Structure and Simulation Methodology

The A/Z graphene SLNRs consist of alternating armchair and zigzag graphene nanoribbons with periodic lengths varying from 0.8 nm to 80 nm. A schematic A/Z graphene SLNR is shown in Fig. 1. All nanoribbons have the similar length of about 80 nm. The 5-7-5 ring topological heterojunction is used for A/Z graphene SLNRs since this heterojunction has been proved to be more stable than other A/Z heterojunction structures [24].

The interactions between C/C, C/H, and H/H atoms in the A/Z graphene SLNRs are described by Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [25, 26]. This potential is widely used to study lattice dynamics and phonon thermal transport of carbon-related nanomaterials, such as graphene and graphyne with optimized parameters [26].

All molecular dynamics (MD) simulations were performed by LAMMPS package [27]. The velocity Verlet algorithm was used to integrate the equations of motion. A time step of 0.55 fs was chosen. The periodic boundary condition was applied along longitudinal direction, and free boundary conditions were applied along the other two directions. The Nosé–Hoover thermostat [28] was employed to control the temperature. All molecular systems were relaxed with *NPT* (constant particle number, pressure, and temperature) ensemble for 200 ps. The constant pressure (1 atm) and temperature (300 K) were kept during this process. After the *NPT* relaxation, the system was relaxed with an *NVE* (constant volume without a thermostat) ensemble for 200 ps. The total energy and temperature of the whole system were monitored during this stage to make sure that the system reached the equilibrium state. At last, a stable structure of A/Z graphene SLNRs was obtained.

Following equilibration, NEMD was performed to compute the thermal conductivity of the A/Z graphene SLNRs. The Muller–Plathe method was employed to impose constant heat flux [29]. The A/Z graphene SLNR was divided into slices in the longitudinal direction. By exchanging the kinetic energies between "hot slab" and "cold slab" on both ends every few steps, a constant heat flux can be applied to the system and a temperature gradient along the heat flux direction was induced. The thermal conductivity of A/Z graphene SLNRs was finally calculated by the Fourier's law

$$\kappa = -\frac{J_L}{\partial T/\partial z},\tag{1}$$



Fig. 2 Dependence of thermal conductivity of A/Z graphene SLNRs on periodic length. The thermal conductivities of armchair and zigzag graphene nanoribbons with same total length and lateral width are also shown for comparison by red and blue solid lines, respectively (Color figure online)

where J_L is the heat flux and $\partial T / \partial z$ is the temperature gradient along the longitudinal direction. In our simulations, it typically took around 0.5 ns to get stable temperature profile. Once reaching the steady state, additional 3 ns simulation was performed to collect data. The thermal conductivity was computed by Eq. 1 overall the collected data.

3 Simulation Results and Discussion

3.1 Thermal Conductivity Dependence of Periodic Length

The dependence of the thermal conductivity of A/Z graphene SLNRs on the periodic length is shown in Fig. 2. The thermal conductivities of armchair and zigzag graphene nanoribbons with same total length and width are also shown for comparison. Figure 2 reveals that the thermal conductivity of A/Z graphene SLNRs is remarkably smaller than that of armchair and zigzag graphene nanoribbons. The thermal conductivity of A/Z graphene SLNRs reduces as much as 87 % compared to that of zigzag graphene nanoribbons, which makes A/Z graphene SLNRs a potential nanomaterial for high-efficiency thermoelectrics. Similar to the previous simulations and experiments [23, 30, 31], the nonmonotonic variation of thermal conductivity of A/Z graphene SLNRs with the periodic length is revealed, which verifies our results. A minimum thermal conductivity for the A/Z graphene SLNRs of 55 W·mK⁻¹ is obtained at the periodic length of 6 nm.

3.2 Mechanism: Vibrational Density of States and Normal-Mode Analysis

In order to reveal underlying mechanism of phonon transport in A/Z graphene SLNR structures, the vibrational density of states (VDOS) [32] for SLNRs is calculated, as



Fig. 3 Comparison of phonon vibrational density of states of interface region and normal region in A/Z graphene SLNR

shown in Fig. 3. VDOS can describe the phonon modes distribution. In order to obtain VDOS, the velocity autocorrelation function is calculated by

$$C(t) = \frac{\langle v(t) \cdot v(0) \rangle}{\langle v^2(0) \rangle},\tag{2}$$

where $\langle v(t) \cdot v(0) \rangle = \lim_{\tau \to \infty} \frac{\int_{-\tau}^{\tau} v(t+t')v(t')dt'}{\int_{-\tau}^{\tau} dt'}$ and VDOS can be computed by

$$C_{vv}(\omega) = \sum_{k=x,y,z} \sum_{j=0}^{N} \int_{0}^{\infty} \frac{\left\langle v_{j}^{k}(t) \cdot v_{j}^{k}(0) \right\rangle}{\left\langle v_{j}^{k}(0) \cdot v_{j}^{k}(0) \right\rangle} e^{i\omega t} dt,$$
(3)

where v_j^k is the velocity component of the *j*th atom along the *k* direction, *j* sums overall the atoms, *k* is a Cartesian direction and sums over *x*, *y*, and *z*; ω is frequency.

The VDOS of atoms located in interface and normal region is shown in Fig. 3. It can be seen that the VDOS of normal region has two peaks which are located at 21 THz and 53 THz, respectively. In contrast, only one high-frequency peak is found at 57 THz in the VDOS of interface region, and no low-frequency peak present. It should also be noticed that the interface region has more scattered distribution of phonon than normal region when the frequency is between 0 THz and 25 THz, which indicates in this frequency range the VDOS of interface region exhibits nonmonochromatic characteristics. Based on phonon theory, the nonmonochromatic phonons could result in the increase in anharmonic effect in the heat conduction, and the thermal conductivity of the system could be reduced [32]. Therefore, the variation of VDOS in Fig. 3 indicates that the interface could reduce thermal conductivity.



Fig. 4 Regional mode weight factor for A/Z graphene SLNRs with different periodic lengths

To understand why the thermal conductivity of A/Z graphene SLNR increases with the decreasing of short periodic length less than 6 nm shown in Fig. 2, we calculate the mode weight factor [33]

$$f_{j,\lambda} = \sum_{j} \sum_{\alpha} \left(\varepsilon_{j\alpha,\lambda} \right)^2, \tag{4}$$

where $\varepsilon_{j\alpha,\lambda}$ presents the vibrational eigenvector components, α is a Cartesian direction, λ is phonon mode, *j* sums over the all atoms in the interface, interior or surface region. In the whole SLNR structure, the sum of the mode weight factors for three regions is equivalent to 1, i.e., for each mode, $f_{interface,\lambda} + f_{interior,\lambda} + f_{surface,\lambda} = 1$.

Figure 4 shows the mode weight factor for A/Z graphene SLNR with different periodic length. The periodic length is 2.6 nm and 6 nm, respectively. It can be noticed that the surface region has similar mode weight factor for these two periodic lengths. However, it is obvious that the phonon mode weight factors of the interface and the interior regions become closer with the decreasing of the periodic length. Similar to the previous studies of superlattice structures [23, 34, 35], the coupled phonon vibration reduces the effect of phonon interfacial scattering and improves the heat conduction. In addition, the phenomenon in Fig. 4 also indicates: (1) The effect of interface region decreases, corresponding to the boosting effect of interior region, with the enlargement of periodic length. Since interface region shows weakening effect on thermal conductivities (details can be seen in the analysis of VDOS), this phenomenon will result in the enhancement of thermal conductivities. (2) The localized properties

of phonons exerted in interface and interior region with longer periodic length are more pronounced. Considering the less effective heat transport of localized modes than that of delocalized modes, the stronger localized properties of systems with long periodic length will lead to lower thermal conductivities. (3) The gap between interface and interior regions of long periodic model is larger, which means the difference of phonon properties of two regions in long periodic model is more outstanding. Further, it can enhance the scattering on the interface of the two regions which will eliminate thermal conductivities to some extent. Overall, among the three factors, factor (1) leads to the increase in thermal conductivities. Therefore, it can be expected that with the increase in thermal conductivities. Therefore, it can be expected that with the increase in periodic length, the effects of the three factors will alter, respectively, and the nonmonotonicity of thermal conductivity curve can be understood.

3.3 Effect of Single-Vacancy Point Defect on Phonon Transport

However, as the periodic length is extremely short, the thermal conductivity of A/Z graphene SLNR cannot be reduced further as shown in Fig. 3, which causes a barrier to maximize ZT values of SLNR as a promising high-performance thermoelectric material. To avoid this, point defects are introduced into the SLNR and expect to decrease the phonon tunneling in SLNR and reduce the thermal conductivity. The relation between thermal conductivity of A/Z graphene SLNRs and periodic length under different density of single vacancy defects is shown in Fig. 5. It can be first noticed that the thermal conductivity of A/Z graphene SLNRs decreases as the density of single-vacancy point defect increases, which is in agreement with our previous work [14]. This indicates that the thermal conductivity of nanostructures can be further decreased by phonon scattering introduced by the point defects. The important result in Fig. 5 is that the thermal conductivity of the A/Z graphene SLNRs is decreased further even if periodic length becomes very small. Thus, the single vacancy defect can decrease the phonon tunneling in SLNR. As discussed in our previous study [14], defects make VDOS move toward lower frequency direction. In the defective region, the more localized phonon modes with low frequency could possess larger probability to take part in boundary scattering of phonons than the phonon modes with high frequency, which leads to the reduction of thermal conductivity.

3.4 Zigzag and Armchair Length Dependence

We also investigated the effects of zigzag and armchair length in periodic length on the thermal conductivity of A/Z graphene SLNRs. The A/Z graphene SLNRs with asymmetric armchair and zigzag length were constructed. The periodic length of 20 nm was fixed. The zigzag length varies from 0.24 nm to 19.6 nm, and armchair length varies from 19.76 nm to 0.4 nm. The longitudinal length of all structures was about 80 nm. As shown in Fig. 6a, for small zigzag length (<12 nm), the thermal conductivity of A/Z graphene SLNR is almost invariant. When the zigzag length is larger than 12 nm, the thermal conductivity of A/Z graphene SLNR increases with the increase in the zigzag length. When the zigzag length is larger than 17 nm, the thermal conductivity



Fig. 5 Variation of the thermal conductivity with periodic length in A/Z graphene SLNRs with different single-vacancy point defects



Fig. 6 Thermal conductivity of A/Z graphene SLNRs as a function of length of zigzag part (a) and armchair part (b)

displays much larger increase. The opposite dependence of thermal conductivity of A/Z graphene SLNR on the armchair length is found and shown in Fig. 6b. It indicates that the larger armchair length in periodic length could result in lower thermal conductivity of A/Z graphene SLNR because the thermal conductivity of armchair graphene nanoribbon is smaller than that of zigzag graphene nanoribbon with same total length and lateral width as shown in Fig. 2.

To understand this phenomenon, phonon polarization analysis is performed for the system. According to phonon polarization analysis, the relative contributions of longitudinal, transverse, and flexural modes to the total phonon conduction in twodimensional A/Z graphene SLNR are quantified by using the method proposed recently [36] as

$$J_{left \to right,\alpha} = -\frac{1}{2wd} \sum_{i \in left} \sum_{j \in right} F_{ij\alpha}(\upsilon_{i\alpha} + \upsilon_{j\alpha}), \tag{5}$$



Fig. 7 Variation of relative contribution (percentage) to total heat flux of A/Z graphene SLNRs from longitudinal, transverse, and flexural (out of plane) lattice vibrations with length of zigzag part (a) and armchair part (b)

where $J_{left \rightarrow right,\alpha}$ is the heat flux through an imaginary interface which divides the structure into "left" and "right" sides, *w* is the width of SLNR, *d* is the thickness of SLNR, $F_{ij\alpha}$ is the α -component of force of atom *i* interacting with atom *j*, $v_{i\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *i*, $v_{j\alpha}$ is the α -component of the velocity of atom *j*, and the two sums are taken over atoms *i* and *j* belonging to the group of "left" and "right," respectively. The detailed computation procedure can be found in Ref. [36]. The phonon transport properties of different nanostructures are successfully investigated by this simple method [37–39]

Figure 7 shows the variation of relative contribution to the total heat flux from longitudinal, transverse, and flexural (out of plane) lattice vibrations with length of zigzag part and armchair part in periodic length of A/Z graphene SLNRs. The trend of the out of plane flexural mode contribution with the change of zigzag length in periodic length of SLNRs shown in Fig. 7a is in agreement with the trend gained in the thermal conductivity variation with zigzag length in the SLNRs presented in Fig. 6a. For A/Z graphene SLNRs with smaller zigzag length, the phonon conduction is governed by the longitudinal modes. For the zigzag length smaller than 12 nm, the contribution from all modes does not vary largely. When the zigzag length is larger than 12 nm, the contribution from the longitudinal modes gradually decreases and at while the contribution from the out of plane flexural modes gradually increases. When the zigzag length is larger than 17 nm, the contribution from the longitudinal modes decreases significantly and the contribution from the out of plane flexural modes increases strongly. At last, the flexural vibrations have the biggest contribution to the total thermal conduction, indicating that the phonon conduction in A/Z graphene SLNR is governed by the flexural modes, which is similar to previous investigations on graphene sheet [40, 41]. The opposite trend of variation of relative contribution to the total heat flux of A/Z graphene SLNR on the armchair length is obtained and shown in Fig. 7b. Figure 7 indicates that the longitudinal modes and the flexural modes competitively govern the phonon conduction of A/Z graphene SLNR with larger zigzag length.

4 Conclusions

In this work, we have investigated the thermal transport properties of A/Z graphene SLNRs by performing nonequilibrium molecular dynamics simulations. The simulation results reveal that the thermal conductivity of A/Z graphene SLNRs depends nonmonotonically on periodic length, which is mainly due to the alteration of localized properties of phonon in interface and interior regions. In addition, we found that introducing single-vacancy point defects into the superlattice nanoribbons can further reduce the thermal conductivity of A/Z graphene SLNRs with the length of zigzag part in periodic length is found. Based on phonon polarizations, relative contributions from longitudinal, transverse, and flexural (out of plane) lattice vibrations are quantified. It is found that the longitudinal modes and the flexural modes competitively govern the phonon conduction of A/Z graphene SLNR with larger zigzag length.

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