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Effect of triangular vacancy defect on thermal conductivity and thermal rectification in graphene nanoribbons

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ABSTRACT

We investigate the thermal transport properties of armchair graphene nanoribbons (AGNRs) possessing various sizes of triangular vacancy defect within a temperature range of 200–600 K by using classical molecular dynamics simulation. The results show that the thermal conductivities of the graphene nanoribbons decrease with increasing sizes of triangular vacancy defects in both directions across the whole temperature range tested, and the presence of the defect can decrease the thermal conductivity by more than 40% as the number of removed cluster atoms is increased to 25 (1.56% for vacancy concentration) owing to the effect of phonon–defect scattering. In the meantime, we find the thermal conductivity of defective graphene nanoribbons is insensitive to the temperature change at higher vacancy concentrations. Furthermore, the dependence of temperatures and various sizes of triangular vacancy defect for the thermal rectification ration are also detected. This work implies a possible route to achieve thermal rectifier for 2D materials by defect engineering.

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1. Introduction

Diodes and/or transistors, as the heart of the working electronic equipment and the origin of the development of electronics industry, have been developed. Many electronic devices based on them are applied in circuit. Similar to electronic counterpart, some novel thermal control and management devices have been proposed [1,2], where one of aims is to solve the global energy problem. In recent years, the research on graphene with two-dimension honeycomb lattice structure of sp^2 bonded carbon atoms has attracted immense attention owing to its ultra-high thermal conductivity which is up to 5300 $W\,m^{-1}\,K^{-1}$ [3,4]. The thermal (phononic) devices based on graphene such as thermal memory [5], thermal transistor [6], thermal logic gate [7] and thermal rectifier [8] are designed to take control of heat flow. Furthermore, the development of these heat-related technologies guides us in working out the puzzle of heat dissipation which is one of the most important barriers to break through. Thermal rectifier, which is similar to electronic rectifier, is deemed as an ideal candidate to solve the problem and to prolong the lifetime of thermal devices. The phenomenon of thermal rectification is that heat flux runs preferably in one direction and inferiorly in reverse direction. So far, most of the researches on thermal rectifiers are based on asymmetric shape [9], inhomogeneous mass interface [10], doped atomic arrangement [11] and atomic defects arrangement [12].

During the synthesis, processing and integration of graphene, we all know that it is difficult to obtain a perfect graphene due to manufacturing constraints, so graphene inevitably exists various defects, such as point vacancy, double vacancy, Stone–Thrower–Wales defect, impurities, antidots [13] and other non-topological structural defects. Many scholars have noted that the various defects in GNRs have important influences on the heat transfer characteristics and get many influential conclusions. Eric Cockayne [14] studied vacancy defects in GNRs. They described seven types of vacancy defects in GNRs. These vacancy defects can occur naturally and also occur by induced. They found that the existence of vacancy defects in GNRs can make it more flexible to avoid a tear or rupture. Wang et al. [12] investigated thermal rectification effect in asymmetrically defected GNRs. They demonstrated optimum conditions for high thermal rectifying efficiency of the thermal rectifier proposed in their work. Yang et al. [11] investigated the thermal conductivity and thermal rectification of triangular single-nitrogen-doped graphene (SNDG) and parallel various-nitrogen-doped graphene (VNDG) by non-equilibrium molecular dynamics. They found the thermal conductivity depends on geometric variations of doped nitrogen and temperature. Thermal rectification of the SNDG decrease with an increasing temperature

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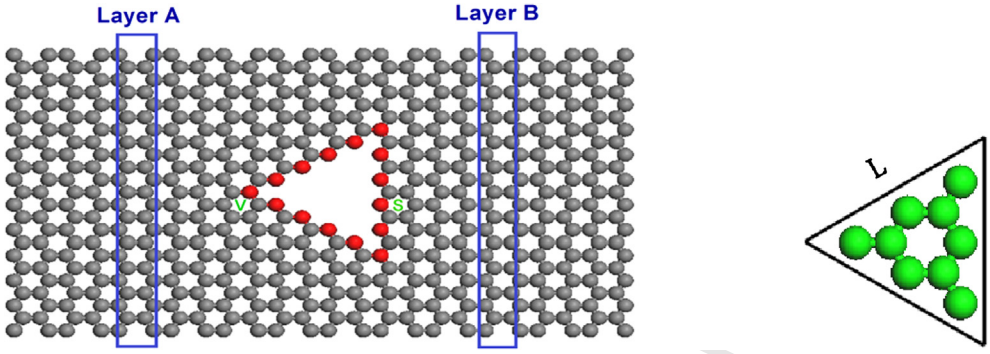

Fig. 1. AGNRs with triangular vacancy defect and removed cluster atoms, respectively. The power spectra are recorded at A and B layers. L is the edge length of triangular vacancy defect.

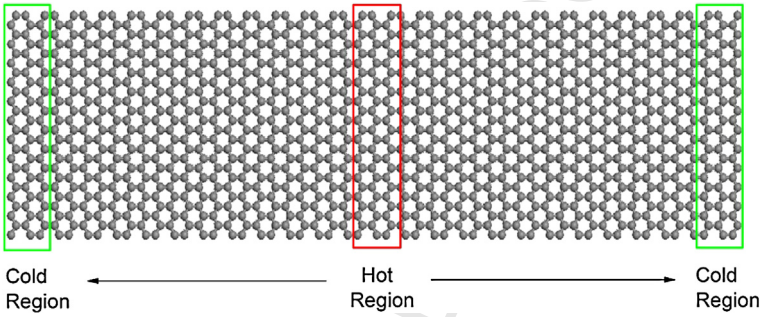

Fig. 2. Schematic of the simulation model for reverse non-equilibrium molecular dynamics. Arrows denote the direction of heat flux.

and that of VNDG remains unchanged. Yang et al. [15] studied the heat flow runs in trapezia-shaped GNR and two rectangular GNRs. They found the flux runs preferentially along the direction of decreasing width and demonstrated excellent thermal rectification efficiency in asymmetric GNRs. Zhang et al. [16] found that there is an obvious thermal rectification ratio in single-layer graphene Y junctions and double-layer Y junctions has a larger rectification ratio than single-layer graphene. Zhang et al. [13] demonstrated a 60–80% reduction of thermal conductivity for different shapes of antidots introduced in AGNRs and ZGNRs.

The aim of this Letter is to perform a more complete insight into the effect of various sizes of triangular vacancy defect (and/or the number of removed cluster atoms) and temperature on the thermal conductivity and thermal rectification of AGNRs by non-equilibrium molecular dynamics. The relationship between these properties was detected.

2. Molecular dynamics modeling

We designed a structure of 21.2 nm long and 3.8 nm wide for AGNRs with triangular vacancy defects (TGNRs). For very narrow GNRs, there is very high concentration of edge defects, and they dominate the thermal transport instead of the asymmetrically introduced triangular vacancy defect. It will affect our results in this study. 3.8 nm wide for AGNRs has negligible size effects on simulation results [12]. Periodic boundary condition was applied in the direction of heat transfer, i.e. the axial direction, which is also along the length of the GNRs. The schematic for AGNRs with triangular vacancy defect and removed cluster atoms are shown in Fig. 1. L is the edge length of triangular vacancy defect. Triangular vacancy defect is in the center of axial direction and width direction.

In this simulation, the velocity Verlet algorithm is used to integrate the motion equations with a time step of $\Delta t = 0.5$ fs. The equilibrium is reached by the constant pressure and constant temperature (NPT) under the Nosé–Hoover thermostats [17,18] for 4×10^5 time steps. Then, the system is switched to NVE ensemble for 1 ns. The thermal conductivity of the graphene nanoribbons was calculated using reverse non-equilibrium molecular dynamics (RNEMD) [19,20]. This method is to impose a heat flux across the axial direction to obtain a temperature gradient, as shown in Fig. 2. The whole structural model was divided into 60 slabs in the axial direction, where the first slabs and the 31th slab (the middle slab) are cold region and hot region. The hottest atom in the cold region swaps periodically its energy with the coldest atom in the hot region in order to achieve a temperature gradient.

Here, we can get a statistical time averaged temperature profile, where the jumps at the end and center positions are due to the mismatch between the heat baths and the graphene lattice, along the axial direction for 50 ps time interval, as shown in Fig. 3. The regions, including hot slab, clod slab and the location of defect, were cut out owing to nonlinear effects, and then took two linear parts to fit the temperature gradient. The temperature gradient of the system is the average of that of these two parts, which is shown in Fig. 4. Finally, based on Fourier's law, the thermal conductivity is evaluated as:

$$k = -\frac{\frac{1}{2}\sum_{Ntransfer}(mv_h^2 - mv_c^2)}{2At\frac{\partial T}{\partial z}} \quad (1)$$

where *Ntransfer* is the total number of swaps; m is the atomic mass; v_h is the velocity of the hottest atom in the cold region; v_c is the velocity of the coldest atom in the hot region; A is the cross-sectional area of the direction of heat transport. Here the cross-sectional thickness of the graphene sheet is considered as a single C–C bond length [21]; t is the total simulation time; $\partial T/\partial y$ is the temperature gradient.

We use the adaptive intermolecular reactive empirical bond order (AIREBO) potential [22] which is an extension of the second-generation reactive bond order as implemented in the

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