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Thermal rectification in asymmetric U-shaped graphene flakes

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Abstract. In this paper, we study the thermal rectification in asymmetric U-shaped graphene flakes by nonequilibrium molecular dynamics simulations. The graphene flakes are composed of a beam and two asymmetric arms. It is found that the heat flux runs preferentially from the wide arm to the narrow arm, which indicates a strong rectification effect. The dependence of the rectification ratio upon the heat flux, the length and the width of the beam and the two arms is studied. It shows that the two asymmetric arms play the central role in thermal rectification and a proper design is needed to obtain the maximum rectification ratio. The result suggests a possible route to manage the heat dissipation in U-shaped graphene based nanoelectronic devices that have recently been fabricated.

Keywords: transport processes/heat transfer (theory), heat conduction

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Graphene, a single layer of carbon atoms arranged in a honeycomb lattice, has attracted much interest due to its extraordinary electronic, mechanical and thermal properties which lead to various important potential applications [1]–[5]. Since graphene exhibits much greater electron mobility than silicon as a zero band gap semiconductor, it has been considered as a promising candidate for the post-CMOS (complementary metal–oxide–semiconductor) material to replace silicon which is approaching its fundamental limit [5]. As electronic devices have undergone dramatic miniaturization, heat dissipation has become one of the most important barriers to break through. To achieve better functionality and longer lifetimes for nanoelectronic devices, it is desirable to have an in-depth understanding of the thermal properties of graphene, which has stimulated intense efforts both experimentally [6]–[8] and theoretically [9, 10]. To design a nanoelectronic device with better heat dissipation capacity, one of the most challenging issues is to design thermal rectifiers. Thermal rectification is a phenomenon where the heat flux runs preferentially in one direction and less in the opposite direction [11]–[13]. Thus realization of thermal rectification in graphene has important implications for graphene based devices. In principle, an asymmetric geometric shape can introduce asymmetric boundary scattering of phonons, whereby the thermal conductivity can be higher along one specific direction and lower in the opposite direction. Thus through molecular dynamics simulations, researchers have proposed several different thermal rectifiers using asymmetric graphene, such as asymmetric rectangular graphene flakes, trapezia-shaped and triangle-shaped graphene flakes, etc [14]–[17]. However, one issue that still remains is how to realize thermal rectification in commonly used structures, such as U-shaped structures. It is known that in nanoelectronic designs U-shaped devices are often used as electronic transistors and logic gates. Thus it is desirable to propose thermal rectifiers based upon U-shaped devices which would have a quite helpful application value. Furthermore, very recently U-shaped graphene flakes have also been fabricated experimentally by using a gallium focused ion beam to cut the U-shaped structures from continuous graphene sheets [18]. It is found that they reveal extremely high $I_{\mathrm{on}}/I_{\mathrm{off}}$ ratios as channel transistors and they can easily realize and control resonant tunneling without any external gates [18, 19]. The promising electronic properties of U-shaped graphene indicate a great application potential in nanoelectronic design. Therefore there is great interest in designing thermal rectifiers using U-shaped graphene flakes.

Here we study the thermal rectification in asymmetric U-shaped graphene flakes by NEMD (nonequilibrium molecular dynamics) simulations. The graphene flakes are composed of a beam and two asymmetric arms. It is found that higher thermal conductivity is obtained when the heat flux runs from the wide arm to the narrow arm. The dependences of the rectification ratio upon the heat flux, the length and the width of the beam, and the length and width of the two arms are studied respectively. It is found that the rectification ratio is not very sensitive to the heat flux. A larger rectification ratio is obtained by decreasing the length or increasing the width of the beam. A particular length difference ratio of the two arms would bring the maximum rectification ratio while the width difference ratio of the two arms would monotonically increase the rectification ratio. Our results may inspire experimentalists to realize thermal rectification in U-shaped graphene flakes.

In figure 1 we show the structure of a U-shaped graphene flake. The graphene flake is composed of a beam and two arms. The bonds of the carbon atoms in the beam are

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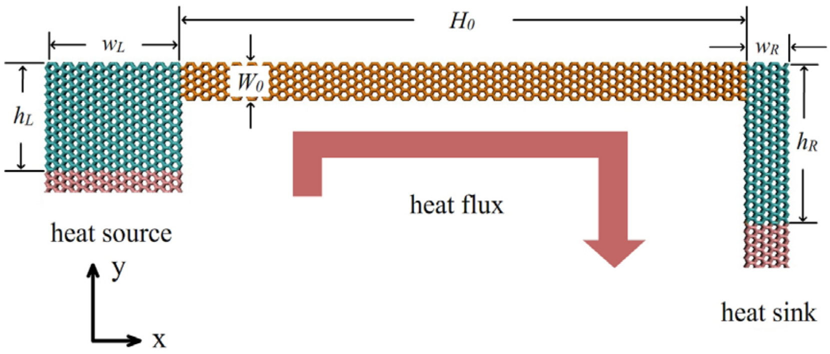

Figure 1. Schematic of a U-shaped graphene flake. The graphene flake is composed of a beam and two arms. The heat source and heat sink are connected to the two arms. The bonds of the carbon atoms in the beam are drawn in orange color. The bonds of the carbon atoms in the left arm and the right arm are drawn in cyan color. The bonds of the carbon atoms in the heat source and heat sink are drawn in red color. The heat flux runs from the heat source to the heat sink.

drawn in orange and the beam has a length of H_0 and a width of W_0. Different H_0 and W_0 are applied to investigate the dependence of the thermal rectification ratio upon the size of the beam. The bonds of the carbon atoms in the left arm are drawn in cyan and the left arm has a length of h_{L} and a width of w_{L}. The bonds of the carbon atoms in the right arm are also drawn in cyan and the right arm has a length of h_{R} and a width of w_{R}. Different ratios of $h_{\mathrm{R}}/h_{\mathrm{L}}$ and $w_{\mathrm{R}}/w_{\mathrm{L}}$ are applied to investigate the dependence of the thermal rectification upon the structural asymmetry. The ends of the two arms are connected with either the heat source or the heat sink. The bonds of the carbon atoms in the heat source and heat sink are drawn in red. Their outmost edges are frozen, which corresponds to the fixed boundary condition. The heat flux runs from the heat source to the heat sink. We use the same reactive empirical bond-order (REBO) potential [20] as implemented in the LAMMPS [21] code to simulate the anharmonic coupling between the carbon atoms. The anharmonic valence-bonded C–C interaction potential consists of a repulsive and an attractive part:

$$E(r_{ij}) = V_{\mathrm{R}}(r_{ij}) - b_{ij}V_A(r_{ij}). \tag{1}$$

Here $V_{\mathrm{R}}(r_{ij}) = (1+Q/r_{ij})A\,\mathrm{e}^{-\alpha r_{ij}}$, $V_A(r_{ij}) = \sum_{n=1,3} B_n\,\mathrm{e}^{-\beta_n r_{ij}}$, r_{ij} is the distance between the carbon atoms, b_{ij} is a function of the local coordination and bond angles for the ith and jth atoms, A, Q, B_n, β are parameters which have been fitted according to carbon systems and can be found in the original paper [20]. The equations of motion are integrated with the velocity Verlet algorithm with the minimum timestep $\triangle t = 0.25$ fs.

First the graphene flakes are equilibrated at a constant temperature $T = 300$ K in a Nosé–Hoover thermostat for 0.75 ns. After that the heat flux is imposed in the graphene flakes running from the heat source to the heat sink. It is realized by the energy and momentum conserving velocity rescaling algorithm developed by Jude and Jullien [22] which is widely used to investigate thermal rectification in different materials [23]–[25]. By rescaling the atomic velocities at each time step dt, a specific amount of kinetic energy $\mathrm{d}E$ is added in the heat source and removed in the heat sink respectively. The heat flux can be calculated by $J = \mathrm{d}E/\mathrm{d}t$. The temperature profiles of the beam and the two arms

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are obtained by dividing the graphene flake into several slabs of constant length 4 Å along its axis. The local temperature of each slab is derived from the averaged kinetic energy. We average the temperature profiles over 100 ps after the heat flux is imposed. After 2 ns the temperature profiles do not change much and the whole nonequilibrium simulation process covers 3 ns.

The heat flux runs from the heat source to the heat sink along the U-shaped graphene flakes. We label the heat flux as J_+ ($J_+ > 0$) when the heat source is connected to the left arm and the heat sink is connected to the right arm. Similarly we label the reversed heat flux as J_- ($J_- < 0$) when the heat source is connected to the right arm and the heat sink is connected to the left arm. If a strong thermal rectification effect occurs in the asymmetric U-shaped graphene flakes, we would obtain different temperature profiles by simply reversing the heat flux. According to Fourier's law, the thermal conductivity of the U-shaped graphene flakes can be given as

$$G_+ = \frac{J_+/A}{\triangle T_+/L} \qquad G_- = \frac{J_-/A}{\triangle T_-/L}. \tag{2}$$

Here A is the averaged cross section of the graphene flakes, L is the distance between the two arms, $\triangle T_+$ ($\triangle T_-$) is the temperature difference between the left arm and the right arm when J_+ (J_-) is imposed. Since $J_+ = -J_-$, A and L are the same, so the thermal rectification ratio η can be given as [11, 23, 24, 26]

$$\eta = \frac{G_+ - G_-}{G_-} = \left(\frac{-\triangle T_-}{\triangle T_+} - 1\right) \times 100\%. \tag{3}$$

In figure 2 we show typical temperature profiles on the beam and the two arms. Here $J_\pm = \pm 0.1$ eV ps^{-1}, $H_0 = 156.6$ Å, $W_0 = 9.7$ Å, $h_\mathrm{L} = 27.9$ Å, $w_\mathrm{L} = 36.4$ Å, $h_\mathrm{R} = 54.6$ Å, $w_\mathrm{R} = 4.0$ Å. The axis of the beam is in the x-axis while the axes of the two arms are in the y-axis. As shown in figure 2(a), there is no obvious difference between the two temperature profiles on the beam by imposing the heat flux J_+ and J_- respectively. Meanwhile, as shown in figure 2(b), distinctively different temperature drops between the two arms are observed by imposing the heat fluxes J_+ and J_- respectively. The temperature drop is much smaller by imposing the heat flux J_+. The different temperature drops on the two asymmetric arms indicate the occurrence of a strong thermal rectification effect by simply reversing the direction of the heat flux. The smaller temperature drop observed when J_+ is imposed indicates that the heat flux runs preferentially from the left arm (the wide arm) to the right arm (the narrow arm). Since the different temperature drop occurs on the two arms rather than the beam, thus it implies that the heat flux runs almost equally along the beam without any preferred direction. The temperature profiles observed illustrate that the thermal rectification effect is caused by the asymmetric arms rather than the beam between them. It gives a hint that the two asymmetric arms would play the dominant role in determining the rectification ratio while the beam would only play the secondary role.

Due to the asymmetric boundary scattering of phonons, a strong thermal rectification effect is observed in U-shaped graphene flakes. In order to illustrate the microscopic mechanism leading to the thermal rectification, i.e., the asymmetric scattering of phonons, we calculate the phonon spectra of two groups of carbon atoms in the U-shaped graphene flakes. The phonon spectrum is derived from the Fourier transform of the velocity

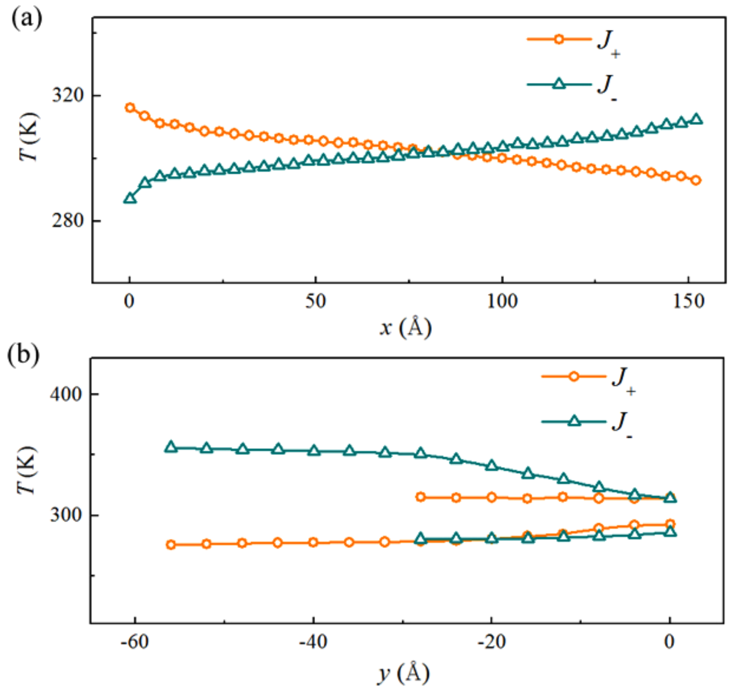

Figure 2. (a) Typical temperature profiles on the beam. It can be seen that there is no distinctive difference between the two profiles by imposing two oppositely directed heat fluxes. (b) Typical temperature profiles on the two arms. The left arm is the short arm and the right arm is the long arm. It can be seen that different temperature drops occur between the ends by imposing two oppositely directed heat fluxes. The result indicates a strong thermal rectification effect.

correlation function which elaborates the vibration properties of the associated atoms in the thermal conduction process [12, 15, 23], [27]–[30]. The phonon spectrum is defined according to the velocities of the carbon atoms $v(t)$ as

$$P(\omega) = \int_0^\infty \mathrm{e}^{-\mathrm{i}\omega t} \langle v(t) \cdot v(t) \rangle \, \mathrm{d}t. \tag{4}$$

Here, $\langle \cdots \rangle$ denotes averaging the carbon atoms in the same layer over velocity v at simulation time t. Here we calculate the phonon spectra of two layers of carbon atoms on the two arms close to the heat baths. The sample velocities are taken from simulation every 1 fs and the correlation is performed over a maximum time interval of 5 ps.

The calculated spectra of the carbon atoms for both heat fluxes J_+ and J_- are shown in figure 3. The mismatches of the phonon spectra indicate the scattering of phonons. To study the underlying properties of the thermal rectification, usually the overlaps of the two spectra are compared for both heat fluxes J_+ and J_- [12, 27, 28, 30]. The difference between the two overlaps corresponds to the rectification phenomenon. It can be seen that there is more overlap areas of the two spectra under J_+ than J_-. The difference in the overlap areas of the phonon spectra indicates that phonons can go through the U-shaped graphene flake more easily under J_+ than J_-. The asymmetric scattering properties of

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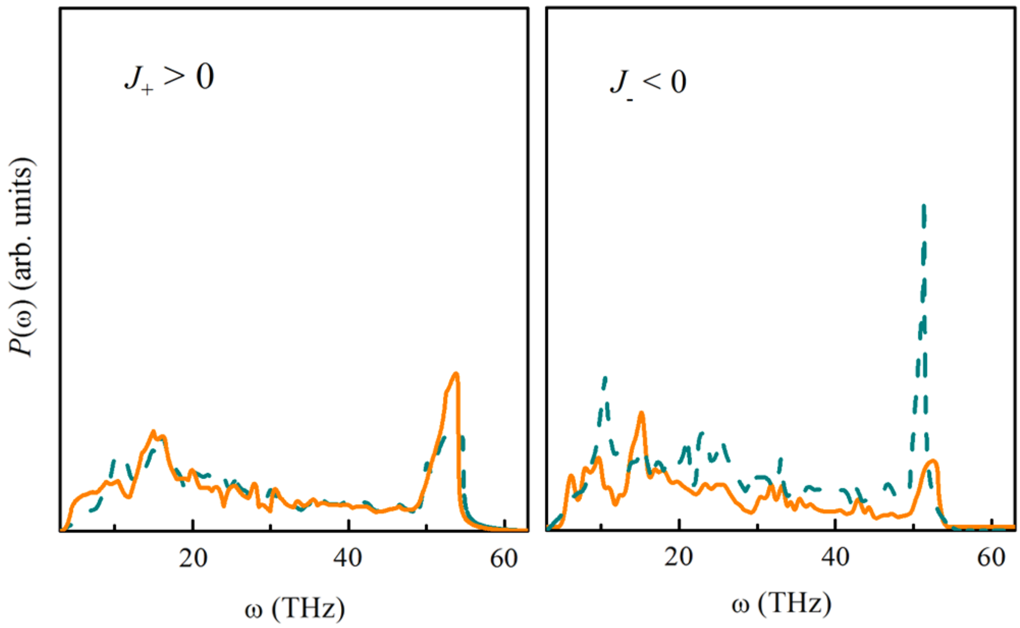

Figure 3. The phonon spectra of the two layers of carbon atoms on the two asymmetric arms close to the heat baths. The phonon spectra of the carbon atoms on the left (wide) arm are drawn with solid orange lines. The phonon spectra of the carbon atoms on the right (narrow) arm are drawn with dashed cyan lines. Both heat fluxes J_+ and J_- are considered. The different overlaps of the two phonon spectra under J_+ and J_- bring different thermal conductivity, thus this is the underlying mechanism of the thermal rectification effect.

the phonons bring the different thermal conductivities of the U-shaped graphene flakes, thus leading to the observed thermal rectification effect.

Very recently, a new theoretical work presented the sufficient conditions for thermal rectification in general graded systems [31]. As long as a local temperature gradient can be built during the thermal conduction process in a graded anharmonic system (such as a structure graded system or a mass graded system, etc), thermal rectification can be observed. Such conditions are quite general for anharmonic crystal models and always happen if Fourier's law holds (but it is not necessary required). In the asymmetric U-shaped graphene flake, the interaction potential is anharmonic between the carbon atoms as shown in equation (1) [20]. The left arm is always wider than the right arm and the temperature profiles in figure 2 indicate that a local temperature gradient can be built. So the asymmetric U-shaped graphene flake can be treated as one of the simplified structure graded models which fulfil the requirements for thermal rectification. Thus another additional explanation of the observed thermal rectification effect is presented from a different aspect.

In order to illustrate the dependence of the rectification ratio upon the heat flux, different heat fluxes are imposed on the graphene flakes. In figure 4(a) we show the heat fluxes $J_\pm$ versus the temperature differences $\triangle T_\pm/T$ between the two arms. It can be seen that the decrease of the temperature difference under J_- is steeper than the corresponding increase of the temperature difference under J_+. The heat flux would run

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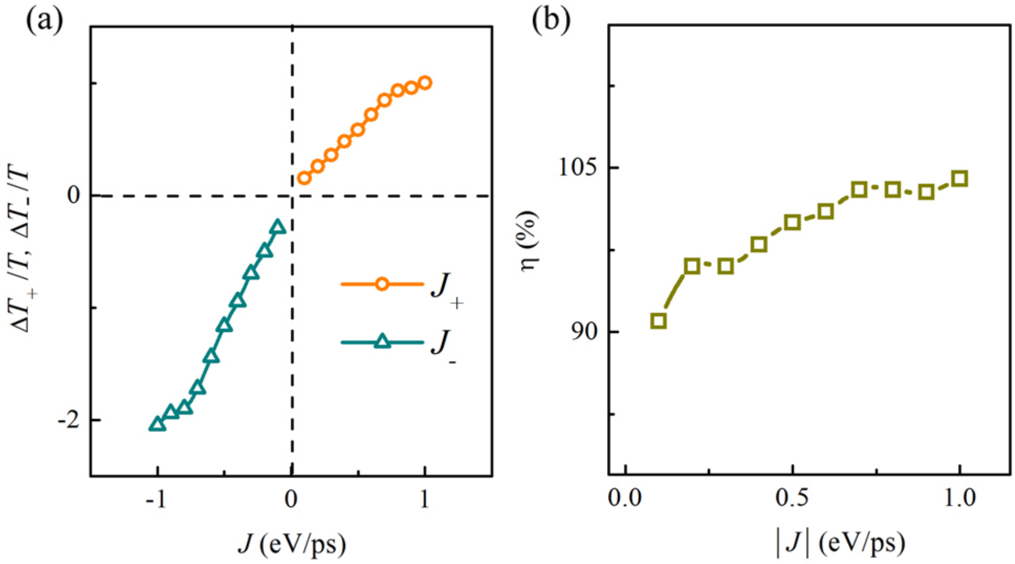

Figure 4. (a) The heat fluxes $J_\pm$ versus the temperature differences $\triangle T \pm /T$ between the two arms. Here J_+ corresponds to $\triangle T_+ > 0$ and J_- corresponds to $\triangle T_- < 0$. The different values of the slopes indicate a strong thermal rectification effect. (b) The thermal rectification ratio η versus the heat fluxes J. The result illustrates that the rectification ratio is not very sensitive to the heat flux.

preferentially from the wide arm to the narrow arm along the graphene flake. The result indicates again that the asymmetric U-shaped graphene flake behaves like a good thermal conductor under J_+ and a poor thermal conductor under J_-. The result is similar to the rectification effect observed in asymmetric graphene nanoribbons and asymmetric carbon nanotubes where the preferred direction is along the direction of decreasing width [14]–[16], [28]. Also, as stated in the theoretical work on ubiquitous thermal rectification in graded systems [31], it is analytically shown that the preferred direction would be along the direction of the grade. The heat flux runs preferentially from the larger part to the smaller part. The result in an asymmetric U-shaped graphene flake as a simplified model of a structure graded system also agrees with that deduction.

In figure 4(b) we show the quantitative dependence of the thermal rectification ratio on the heat flux. It shows that although the increase of the heat flux results in increase of the rectification ratio the rectification ratio is not very sensitive to the heat flux. With $J_\pm = \pm 0.1$ eV ps^{-1} the rectification ratio is 91%, while with $J_\pm = \pm 1.0$ eV ps^{-1} the rectification ratio increases to 104%. This indicates that the thermal rectification effect in asymmetric U-shaped graphene flakes is mainly dependent upon the asymmetry of the structure and insensitive to the generated heat or environmental temperature. The result demonstrates that the U-shaped graphene flakes have an obvious advantage in real applications for nanoelectronic devices. A large rectification ratio could still be expected even only small amount of heat flux is generated in these devices.

In order to investigate the influence of the beam on the thermal rectification, different lengths and widths of the beam are studied. The two arms are kept invariant to keep the same structural asymmetry and $J_\pm = \pm 0.6$ eV ps^{-1} is implemented. In figure 5(a) we show

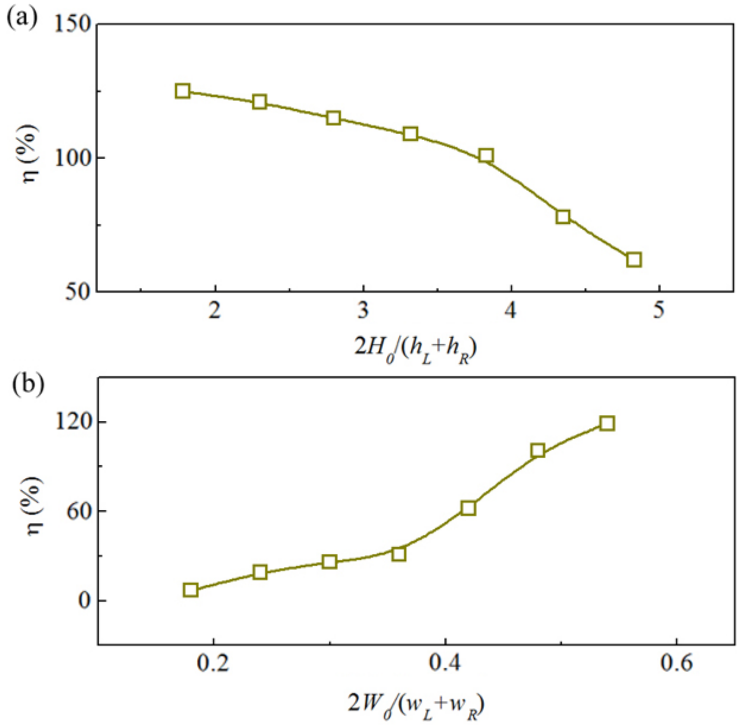

Figure 5. (a) The dependence of the thermal rectification ratio η on the length of the beam. The result indicates that the rectification ratio is gradually decreased with the length of the beam. Here $(h_\mathrm{L}+h_\mathrm{R})/2 = 40.9$ Å and H_0 varies from 72 to 197 Å. (b) The dependence of the thermal rectification ratio η on the width of the beam. The result indicates that the rectification ratio would be greatly decreased by decreasing the width of the beam. Here $(w_\mathrm{L}+w_\mathrm{R})/2 = 20.2$ Å and W_0 varies from 3.6 to 10.9 Å.

the dependence of the rectification ratio on the length of the beam. The result indicates that although the rectification effect is enhanced by decreasing the length of the beam, it is not very sensitive to the length of the beam. For example, even if the length of the beam is much longer than the average length of the two arms $(H_0/((h_\mathrm{L}+h_\mathrm{R})/2) = 4.83)$, the rectification ratio η only decreases to 62%. In figure 5(b) we show the dependence of the rectification ratio on the width of the beam. The result indicates that the rectification effect would be greatly weakened by decreasing the width of the beam. For example, when the width of the beam is small enough $(W_0/((W_\mathrm{L}+W_\mathrm{R})/2) = 0.36)$, the rectification ratio η decreases to less than 31%. Thus the length and the width of the beam play quite different roles in the thermal rectification effect for asymmetric U-shaped graphene flakes.

In order to investigate the effect of structural asymmetry on thermal rectification, different length and width difference ratios of the two arms are also studied. The beam is now kept invariant and $J_\pm = \pm 0.6$ eV ps^{-1} is implemented. In figure 6(a) we show the dependence of the thermal rectification ratio on the length difference ratio between the two arms. The rectification ratio η reaches its maximum value around a length difference ratio of $h_\mathrm{R}/h_\mathrm{L} = 1.91$. The result shows that although the length asymmetry increases with h_R or h_L the rectification ratio would be greatly decreased if their length difference

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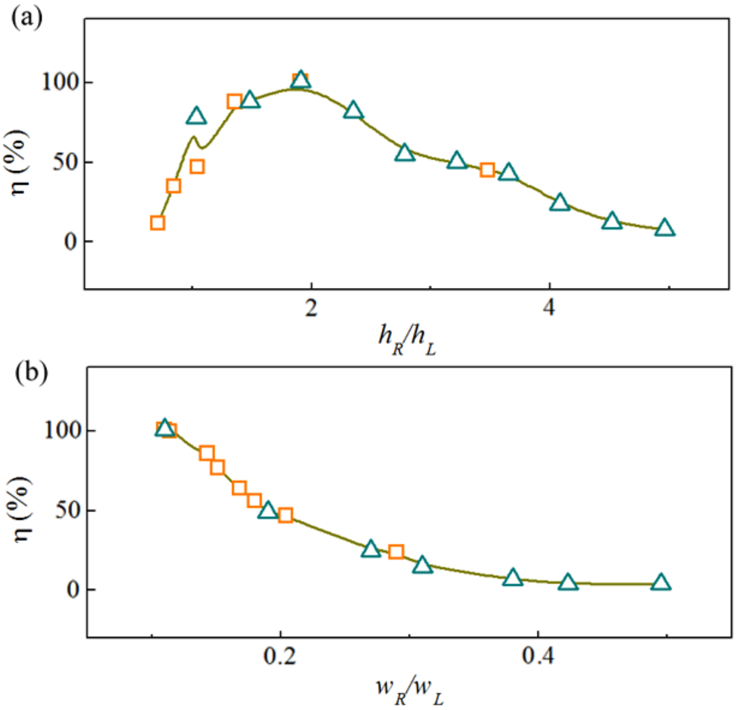

Figure 6. (a) The dependence of the thermal rectification ratio η on the length difference ratio $h_{\rm R}/h_{\rm L}$ between the two arms. The result indicates that the maximum rectification ratio is obtained for a length difference ratio of around $h_{\rm R}/h_{\rm L} = 2$. (b) The dependence of the thermal rectification ratio η on the width difference ratio $w_{\rm R}/w_{\rm L}$ between the two arms. The result indicates that the rectification ratio is monotonically increased with the width difference ratio. (The triangles in (a) and (b) are obtained by varying the right arm. The squares in (a) and (b) are obtained by varying the left arm.)

ratio deviated from the proper value. In figure 6(b) we show the dependence of the thermal rectification ratio on the width difference ratio between the two arms. The rectification ratio would be increased monotonically with the width difference (since $w_{\rm L} > w_{\rm R}$, thus the width difference is greater when $w_{\rm R}/w_{\rm L}$ is smaller). Therefore it can be obtained that in real applications a large rectification ratio would be expected by introducing a more suitable length asymmetry and a large width asymmetry between the two arms.

As stated above, the asymmetric U-shaped graphene flake can be treated as a simplified structure graded model. Thus we can understand the dependence of the rectification ratio on the structural asymmetries according to the associated properties of graded systems in theoretical work [31]. First we discuss how the rectification ratio reaches the maximum value at a proper value of $h_{\rm R}/h_{\rm L}$. For a small value of $h_{\rm R}/h_{\rm L}$ ($h_{\rm R}/h_{\rm L} \sim 0$), either $h_{\rm L} \sim \infty$ or $h_{\rm R} \sim 0$. When $h_{\rm L} \sim \infty$, the contribution of the right arm can be neglected compared with the left arm and the structural grade of the system is greatly reduced. Also the length of the system is enlarged for $h_{\rm L} \sim \infty$. So the rectification ratio which is proportional to the structural grade and inversely proportional to the length of the system would be reduced to a very small value. When $h_{\rm R} \sim 0$, the contribution of the right arm can also be neglected compared with the left arm. The temperature gradient along the right arm only plays an insignificant role then. The heat bath can be seen as directly connected to the beam and the left arm, thus the structural grade of the system is also greatly reduced. So, in this case, the rectification ratio which is proportional to the structural grade would also be reduced to a very small value. For a large value of h_R/h_L ($h_R/h_L \sim \infty$), either $h_L \sim 0$ or $h_R \sim \infty$. Similarly the rectification ratio would also be reduced to a very small value. So this explains why the maximum rectification ratio would be obtained by designing a proper value of h_R/h_L which is neither too small nor too large. Second we discuss how the rectification ratio would be increased monotonically with the width difference $1/(w_R/w_L)$. Since the left arm is always wider than the right arm, the structural grade is proportional to the width difference $1/(w_R/w_L)$. So the rectification ratio which is proportional to the structural grade would also be proportional to the width difference $1/(w_R/w_L)$.

In summary, we designed a thermal rectifier using a U-shaped graphene flake by introducing asymmetric arms. A strong thermal rectification effect is observed and the preferred direction of the heat flux is from the wide arm to the narrow arm. The rectification ratio is not very sensitive to the heat flux which might be important for nanoelectronic devices where only small amount of heat flux is generated. In addition, we state that proper designs of the beam and the structural asymmetries are necessary to obtain the maximum rectification ratio. Our results may be useful for engineering U-shaped graphene based nanoelectronic devices that have recently fabricated and shown promising potential in real applications.

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