

# Thermal conductivity of graphene nanoribbons

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We have investigated the thermal conductivity of graphene nanoribbons (GNRs) with different edge shapes as a function of length, width, and strain using nonequilibrium molecular dynamics method. The initial GNR for the functional variations has dimensions of  $2 \times 11 \text{ nm}^2$ . Strong length dependence of thermal conductivity is obtained, indicating high thermal conductivities of GNRs, which is consistent with the experimental results for graphene. A tensile/compressive uniaxial strain can remarkably decrease the thermal conductivity of GNR. © 2009 American Institute of Physics.  
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Graphene, a single sheet of graphite, has attracted great attention due to its prominent electronic and thermal properties since it first became experimentally accessible in 2004.<sup>1–5</sup> Recently, graphene nanoribbons (GNRs), which are quasione-dimensional graphene nanostructures, became realizable because of the progress in preparing graphene on conventional device setups.<sup>6–9</sup> The electronic, magnetic, and vibrational properties of GNRs have been extensively studied both theoretically and experimentally,<sup>10–18</sup> which indicates that GNRs are promising material for nanoelectronic applications. Owing to the quantum confinement and edge effect, also, GNRs are expected to exhibit some outstanding thermal properties. However, to the best of our knowledge, the thermal properties of GNRs have not been well studied. From a practical point of view, good thermal managements of GNRs have potential applications of future GNR-based thermal devices, which can greatly improve performances of the nano-sized devices due to heat dissipations.

Moreover, as the electronic industry moves toward nanometer designs, the thermal dissipation problem in electronic circuits has become one of the most important challenge.<sup>19</sup> A possible approach for solving the thermal problem is finding a material with high thermal conductivity, which can be integrated with Si complementary metal-oxide-semiconductor (CMOS) technology. Diamond and carbon nanotubes (CNTs) have been considered for such applications.<sup>20,21</sup> However, due to the large thermal contact resistance, they are not well suited for integration with CMOS. Different from the diamond and CNTs, while, GNRs can be naturally attached to heat sinks, and thus avoiding the problem of thermal contact resistance.<sup>5</sup> This suggests GNRs can be excellent material for thermal management in the CMOS devices and circuits. Thus the investigation of thermal conductivity properties of GNRs is greatly desirable.

In this letter, using the nonequilibrium molecular dynamics (NEMD) method,<sup>22</sup> we investigate thermal conductivity of two types of GNRs, i.e., the armchair GNR (AGNR) and the zigzag GNR (ZGNR). The results indicate that the GNRs have very high thermal conductivities and long phonons' mean free paths (PMFPs). It is also found the thermal conductivity is sensitive to the edge shapes, widths, and strains of GNRs. Combined with their unique electronic properties,

GNRs may be a suitable candidate in future CMOS nanodevices.

In the MD simulation, we use Tersoff<sup>23</sup> potential to describe the C–C bonding interactions, and employ the velocity Verlet method to integrate equations of motion with a fixed time step of 0.5 fs. Fixed boundary condition is applied, where the outmost two layers of each head are fixed. Then two layers of each end are put into contact with the Nosé–Hoover heat bathes with temperatures 310 and 290 K, respectively.<sup>24</sup> The thermal conductivity  $K$  is then calculated from the Fourier law,

$$K = - \frac{J}{\nabla T \cdot S}, \quad (1)$$

where  $J$  is the heat flux from the heat bath to the system, which can be obtained via calculating the power of heat baths.<sup>25</sup>  $\nabla T = dT/dx$  is the temperature gradient in the length direction, and  $S$  is the cross-section area. Here we choose  $d = 0.144 \text{ nm}$  as the GNRs' thickness. All results given in this paper are obtained by averaging about  $10^7$  fs after a sufficient long time ( $10^7$  fs) to set up a nonequilibrium stationary state. In addition, all the GNR structures are fully optimized before further NEMD calculations. For convenient representation, we refer to a GNR with  $N$  dimer lines in width as  $N$ -AGNR or  $N$ -ZGNR, depending on the specific edge shapes.<sup>18,26</sup>

We first calculate the thermal conductivity of 20-AGNR and 10-ZGNR with a length ( $L$ ) of 11 nm, both of which have similar width about 2 nm. It is found the thermal conductivity of 20-AGNR is 218 W/m K, much smaller than that of 10-ZGNR (472 W/m K). This indicates an obvious edge-shape dependence of thermal conductivity of GNRs. We also calculated thermal conductivity of armchair and zigzag graphene with the length of 11 nm, by applying a periodic boundary condition in the width direction of 20-AGNR and 10-ZGNR, respectively. While, much higher thermal conductivity values were obtained, where  $K = 460(590) \text{ W/m K}$  for the armchair (zigzag) graphene. This suggests the edge in the GNRs could decrease the thermal conductivity, which can be own to the following two facts. First, compared with that of graphene, there appears two edge-localized phonon modes in the low-energy region for the GNRs, i.e., the transverse acoustic mode, and the lowest-lying optical mode.<sup>15</sup> The edge-localized phonons can interact with other low-energy

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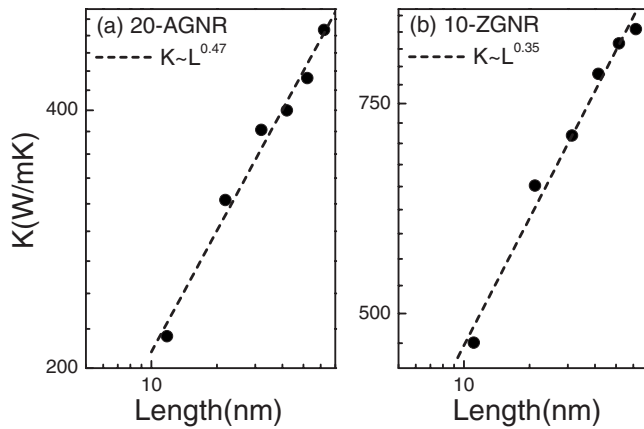


FIG. 1. Thermal conductivity  $K$  vs the length  $L$  in log-log scale for 20-AGNR and 10-ZGNR. In both cases,  $K \sim L^\beta$ , with  $\beta$  being comparable to that of SWCNs. This indicates the GNRs also have very high thermal conductivities and long PMFPs.

phonons and thus reduce their PMFP (edge effect). This would remarkably reduce the low-energy phonons' contribution to the thermal conductivity, which is very substantial and significant for the thermal transport. Second, boundary scattering at the edge of GNRs also reduces the thermal conductivity. Moreover, it is noticed that the thermal conductivity difference between the armchair graphene and 20-AGNR is about 242 W/m K, much larger than that between the zigzag graphene and 10-ZGNR (118 W/m K), implying more significant edge effect in the AGNRs.

The length dependence of thermal conductivity of GNRs, which is very important for the low-dimensional system's thermal-conduction investigations, is also calculated (Fig. 1). From Fig. 1, the thermal conductivity does not converge to a finite value with the increase of GNRs' length up to 60 nm, while follows a power law of  $K \sim L^\beta$ , with  $\beta = 0.47$  and  $0.35$  for the 20-AGNR and 10-ZGNR, respectively. Similar phenomenon has also been observed in the SWCNs, where  $\beta$  varies from 0.3 to 0.4.<sup>27,28</sup> Thus, the strong length dependence of thermal conductivity may also indicate very long PMFPs in GNRs. Based on the scaling rule indicated in Fig. 1, we can also predict the thermal conductivity of GNRs with an experimental length. Through the extrapolation procedure, it is found that the 20-AGNR and 10-ZGNR with a length of 2  $\mu\text{m}$  have thermal conductivities of about 2400 and 3000 W/m K, respectively, indicating the high thermal conductivities of GNRs. Moreover, Ghosh *et al.*<sup>5</sup> have experimentally found that graphene has thermal conductivities in the range of 3000–5000 W/m K depending on the specific sizes, which vary from 1 to 5  $\mu\text{m}$ . Although the simulated GNRs have much smaller width (only 2 nm) than that of the graphene in experiment, we observed the strong size dependence in agreement with Refs. 4 and 5.

As is well known, the electronic properties of GNRs are very sensitive to their widths.<sup>11,12</sup> As for the thermal properties, we can also expect a strong width dependence of thermal conductivity. Figure 2 shows the thermal conductivity of both  $N$ -AGNRs and  $N$ -ZGNRs with variation of  $N$ . As one can see, the ZGNR's thermal conductivity increases first and then decreases with  $N$  increasing, while the AGNR's thermal conductivity monotonously increases with  $N$ . This interesting phenomena can be understood from the following mechanism. On one hand, increasing  $N$  can increase the number of

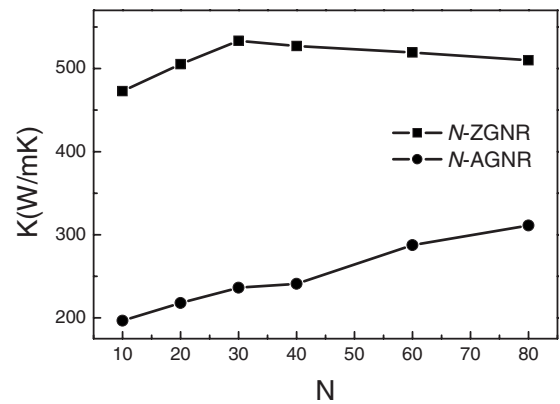


FIG. 2. Thermal conductivity of  $N$ -AGNR and  $N$ -ZGNR with variation of  $N$ , where the length of GNRs is fixed to be 11 nm. The ZGNR's thermal conductivity increases first and then decreases with  $N$  increasing, while, the AGNR's thermal conductivity monotonously increases with  $N$ .

phonon modes of GNRs, while the number edge-localized phonon modes does not change with  $N$ .<sup>15–17</sup> Thus the edge effect on the thermal transport decreases and the thermal conductivity increases with  $N$  increasing. On the other hand, the energy gap between different phonons also decreases with  $N$  increasing. This can increase the probability of phonons' umklapp process and reduce the thermal conductivity.<sup>29</sup> The thermal conductivity variations can be own to such two effects that compete with each other. For the  $N$ -ZGNRs with small  $N$ , the reduction of edge effect is dominate and the thermal conductivity increases with  $N$  increasing. When  $N$  gets large enough, the increase of phonons' umklapp effect would become dominated and the thermal conductivity begin to decrease with  $N$ . Different from that of ZGNRs, however, the edge effect is much more significant in the AGNRs. So the reduction of edge effect is always dominate in the AGNRs, and the thermal conductivity monotonously increases with  $N$  increasing. Such distinct width dependence of thermal conductivity of GNRs with different edge shapes could be particularly important for the GNR-based thermal-material's designations.

In addition, strong size (both length and width) dependence of thermal conductivity of graphene with micrometer size has also been observed by Nika *et al.*<sup>30,31</sup> theoretically. Thus our results indicate the thermal conductivities of GNRs have similar size-dependence trend with that of graphene, although the absolute values are different.

The uniaxial strains can also strongly influence a GNR's thermal conductivity. Shown in Fig. 3 is the tensile/compressive uniaxial strain dependence of thermal conductivities of 20-AGNR and 10-ZGNR. As one can see, the thermal conductivity of 20-AGNR (10-ZGNR) remarkably decreases with the tensile strain increasing, which approaches to an ultima value when the strain gets large enough. Furthermore, the ZGNR's thermal conductivity is more sensitive to the tensile strain than that of AGNR. A huge thermal conductivity reduction of 77% can be obtained with a tensile strain of 16% for the 10-ZGNR, which is much larger than that for the 20-AGNR (with a reduction of 56%). The thermal conductivity reduction under tensile strains can be own to the decrease of the stiffness tensor and the increase of lattice anharmonicity.<sup>32</sup> In contrary to that of conventional materials, the GNRs' thermal conductivity decreases with the compressive strain. This can be contributed

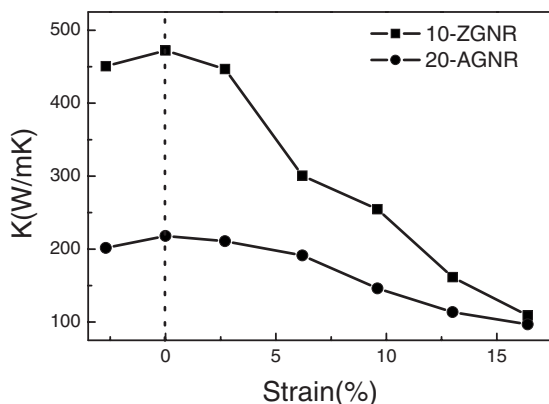


FIG. 3. Uniaxial strain dependence of thermal conductivity of 20-AGNR and 10-ZGNR. The unstrained length is 11 nm. Very remarkable decrease of thermal conductivity is obtained when the tensile/compressive strain is employed.

to the unique geometry of GNRs, where a fluctuant structure would be formed when an uniaxial compressive strain is applied,<sup>33</sup> in which the phonon scattering effect is more prominent than that in a flat structure.

In summary, we have investigated thermal conductivity of GNRs with different edge shapes as a function of the length, width, and strain in use of the NEMD method. The thermal conductivity does not converge to a finite value with the increase of GNRs' length up to 60 nm, while follows a power law of  $K \sim L^\beta$ , indicating very high thermal conductivities and long PMFPs of GNRs. Moreover, the thermal conductivity is very sensitive to the edge shapes. It is found the ZGNR's thermal conductivity increases first and then decreases with the width increasing, while, the AGNR's thermal conductivity monotonously increases with width. A competitive mechanism is further proposed to explain such interesting phenomena. Very remarkable decrease of thermal conductivity is also obtained when a tensile/compressive uniaxial strain is applied on the GNRs.

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