Negative Differential Thermal Conductance in Graphene Nanoribbons: Toward Graphene Thermal Circuits

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Abstract: Graphene has received much attention due to its remarkable electronic properties. It also has exceptional thermal properties, such as an unusually high thermal conductivity. Understanding thermal transport of graphene is of great importance to the applications for future graphene-based devices in energy efficient nanoelectronics. We have calculated the thermal current of symmetric and asymmetric graphene nanoribbons (GNRs) up to large temperature bias and obtained the negative differential thermal conductance (NDTC). We adopt classical molecular dynamics simulation based on the Brenner potential of carbon-carbon bonding with Nosé-Hoover thermostats. For asymmetric GNRs, the NDTC exists only when the temperature at the narrower end is larger than that at the wider end. The NDTC is probably due to the decrease of the thermal conductivity when the average temperature is decreased. A possible thermal amplifier is constructed based on the effect of NDTC. The NDTC in GNRs can have potential applications in nanoscale thermal management. It can also open the possibility to building "thermal logic", using heat as a novel computational variable to process information.

I. Introduction

Graphene, a two dimensional monolayer of honeycomb carbon lattice, has drawn intense attention since its first experimental isolation [Novoselov 2004]. Graphene shows remarkable properties, such as the massless Dirac fermions, anomalous quantum Hall effect and unusual high thermal conductivity [Castro Neto 2009, Balandin 2008, Ghosh 2008]. Graphene nanoribbons (GNRs) are symmetric/asymmetric narrow strips of graphene and considered as basic elements for future nanoelectronics. It has been demonstrated that many properties of GNRs, such as the energy gap and magnetization order, can be tuned by their widths and edge chirality [Nakada 1996, Son 2006, Han 2007, Chen 2007]. Recent studies show that the thermal conductivity of GNRs also depends on their edge chirality from molecular dynamics simulations [Hu 2009] and ballistic phonon transport [Jiang 2009]. For example, GNRs with zigzag edges have larger thermal conductivity than GNRs with armchair edges. The effect of thermal rectification, with larger thermal conductivity in one direction than the opposite direction, has been observed experimentally and theoretically in several carbon based systems [Chang 2006, Wu 2007, Wu 2008, Li 2004]. The lattice nonlinearity (anharmonic effect) plays the essential role in thermal rectification. It has also been found that the negative differential thermal conductance (NDTC) exists in the one dimensional ideal nonlinear lattice [Li 2006]. Based on NDTC, the thermal logic and even thermal memory have been proposed [Wang 2007, Wang 2008]. To the best of our knowledge, NDTC has not been studied in any graphene system. In this work, we have used classical molecular dynamics to study the NDTC in both symmetric and asymmetric GNRs. The NDTC in graphene may have potential application in future thermal logic circuits.

II. Simulation method: nonequilibrium classical molecular dynamics

In our work, we have used the nonequilibrium classical molecular dynamics based on the Brenner potential [Brenner 1990] of carbon-carbon bonds. The lattice nonlinearity has been embedded automatically in the Brenner potential. The GNRs studied in this work are shown in Figure 1.

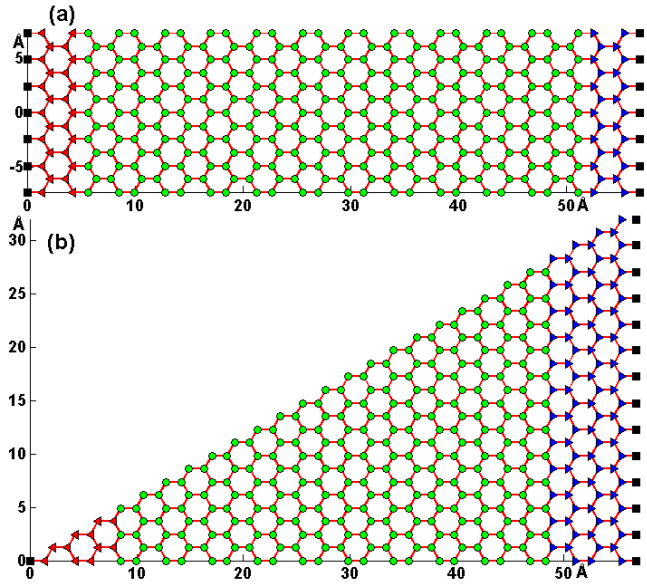

Figure 1. GNRs studied in this work: (a) symmetric rectangular GNR and (b) asymmetric triangular GNR.

In Figure 1, atoms denoted with black squares are fixed. The atoms denoted with left-pointing-triangle and right-pointing-triangle are placed in the Nosé-Hoover thermostats [Nosé 1984, Hoover 1985] at different temperatures. The temperature difference at the two ends of GNRs results in the thermal current along the direction of the temperature gradient. One of the most distinctive differences between the thermal transport and electron transport is that the thermal current depends on not only the temperature difference but also the average temperature because the chemical potential of phonons cannot be controlled. The details of the simulation can be found elsewhere [Hu 2009]. We did not implement the temperature correction in this work.

III. Results and discussions

First, we calculated the thermal current of the symmetric GNR in Figure 1(a) and the results are shown in Figure 2. The temperature at two ends of symmetric GNR is denoted with T_L (left end) and T_R (right end) respectively. In the solid red line of Figure 2(a), T_R is kept as a constant of 300 K and NDTC is obtained when T_L is in the range of 100 - 200 K. For example, the increase of the temperature difference T_R-T_L leads to the decrease of the thermal current. It is noteworthy that the average temperature $(T_R+T_L)/2$ decreases when the temperature difference increases. The NDTC still exists after doubling the length of the GNR, as shown in the dashed blue line of Figure 2(a). In Figure 2(b), T_R is kept at 600 K for the GNR of Figure 1(a) and the NDTC is observed with T_L in the range of 200 - 350 K.

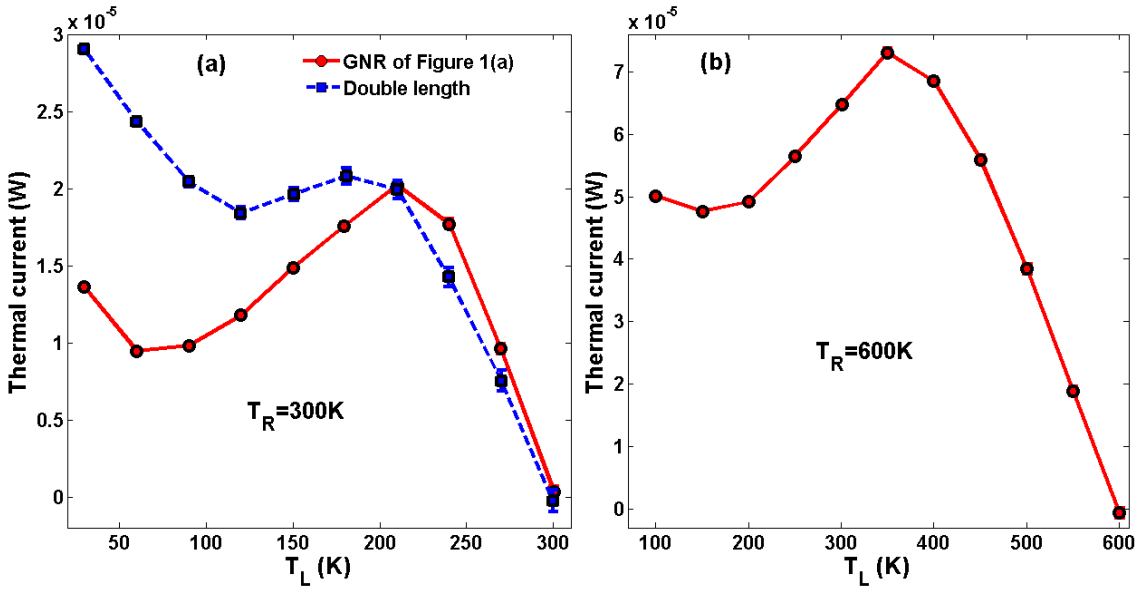

Figure 2. Thermal current of symmetric GNRs.

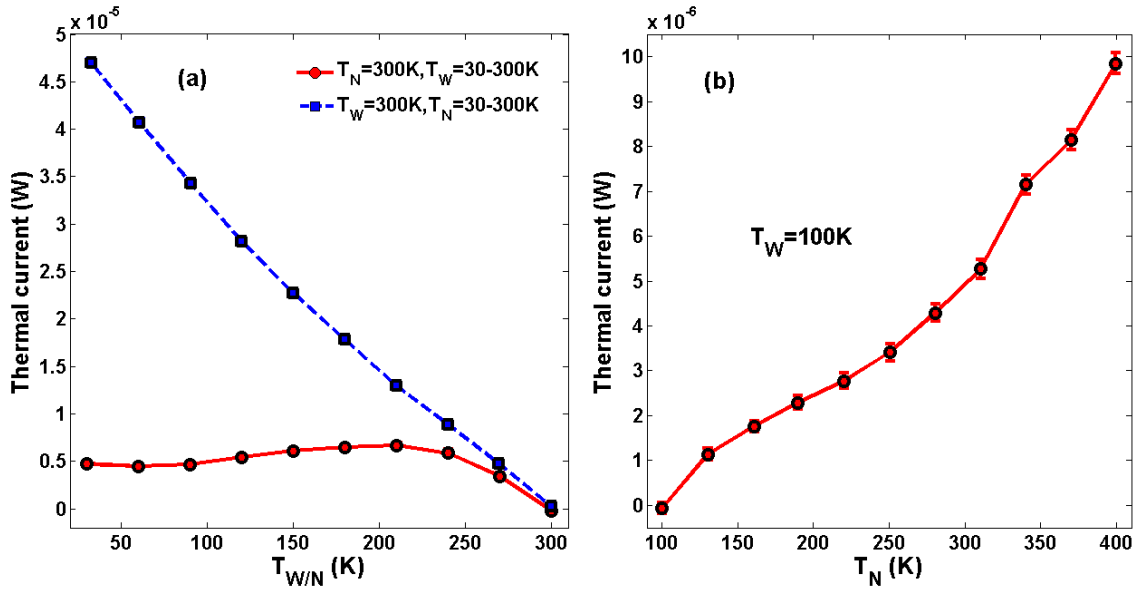

Figure 3. Thermal current of asymmetric GNRs.

For the asymmetric GNR of Figure 1(b), the temperature at the narrower (wider) end is denoted with T_N (T_W). In Figure 3(a), the solid red line shows NDTC with T_W in the range of 100 – 200 K when T_N is kept at 300 K, but NDTC does not exist when T_W is kept at 300K. We noticed that for both the symmetric and asymmetric GNRs, the NDTC exists if the average temperature decreases when the temperature difference increases. In Figure 3(b), T_W is kept at 100 K while T_N is swept from 100 K to 400 K so that T_N is larger than T_W (same as the solid line of Figure 3(a)). However, in Figure 3(b) the average temperature increases when the temperature increases and there is no NDTC. Therefore, we suggest that the NDTC is due to the decrease of the average temperature which can decrease the thermal conductivity of GNRs.

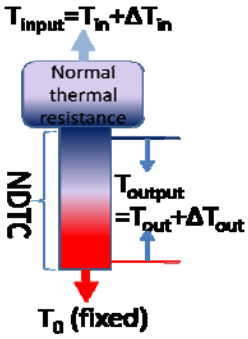

Figure 4. Possible thermal amplifier.

Based on the NDTC of the symmetric GNR, a possible thermal amplifier is shown in Figure 4. Analogous to the simple electrical amplifier based on an negative differential electrical resistance in series with a resistor, we can also find here the amplification factor defined as $A=|\Delta T_{out}/\Delta T_{in}|=(1\text{-}GR)^{-1}$, where G is the magnitude of the NDTC and R is the value of the normal thermal resistance.

IV. Summary

In our work we used classical molecular dynamics to simulate the thermal transport in GNRs up to large temperature bias. The NDTC is observed in both symmetric and asymmetric GNRs. For the symmetric GNR, NDTC exists even the length of the GNR and temperature range are doubled. For the asymmetric GNR, NDTC is obtained only when the thermal current flows from the narrower to the wider end. We suggested that the NDTC is caused by the decrease of the average temperature and the corresponding thermal conductivity. We also proposed a possible thermal amplifier based on the NDTC.

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