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Computation of the thermal resistance in graphene sheets with a rectangular hole

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ABSTRACT

Employing nonequilibrium molecular dynamics (NEMD) simulation method, we have computed the thermal resistance in graphene sheets when a nanosized rectangular defect is embedded in the middle of the system. Simulation results indicate that the thermal resistance is an increasing function of the defect's height (perpendicular to the heat flow direction) but it is virtually insensitive to the defect width. Therefore, the defect height is the key factor in decreasing the thermal conductivity of the defective graphene for thermoelectric applications. Our simulations exhibited two temperature jumps in the temperature profile with the jump near the cold bath being greater than the second one. Furthermore, our results showed that the temperature of the constricted region constructed by the defect was higher than in other regions for narrow constrictions due to thermal energy accumulation and it had a local temperature gradient counter to that of the original temperature. Density of states analysis demonstrates that the thermal resistance in defective graphene is due to phonon scattering at the defect interface.

1. Introduction

With downsizing of micro/nano electronic devices and packaging them in single units, the question of rise in the total thermal energy generation has become inevitable. Device performance and its lifetime would deteriorate if the thermal energy is not extracted quickly [1]. Graphene can be the best candidate for solving the heat dissipation problems because of its excellent thermal conductivity properties [2,3] as well as its flexibility to fashion it into a broad range of geometrical shapes compared with other highly conductive materials. In chemical vapour deposition (CVD) technique for growing graphene on metal foils such as copper and nickel [4,5], grain boundaries are ubiquitous in large graphene sheets because grains in the foil serve as nucleation sites for the graphene. A grain boundary serves as an obstacle to heat transfer [6–8] and promotes thermal boundary resistance, especially when the characteristic length of the system is less than the mean free path of phonon (about 775 nm at room temperature [2]).

Thermal boundary resistance, also known as Kapitza resistance, has been defined as the ratio of the temperature variation at the interface to the heat current across it [9]

$$R = \frac{\Delta T}{J} \quad (1)$$

where ΔT is the temperature change and J is the heat current. The Kapitza resistance is due to two basic factors; namely the different properties of the heat carriers on the two sides of the joint due to difference in the materials, or the structure of two sides [10] and heat carriers scattering [6]. It has been reported that the thermal boundary resistance increases linearly inversely with the system's length [11]. Zhan et al. [12] reported that by controlling the type and distribution pattern of the graphyne or graphyne-like structures that incorporate the graphene nanoribbons (GNRs), thermal properties of GNR become tuneable. It is well-known that the thermal resistance depends on many factors such as material, geometry, temperature, and the system's length. Very recently, thermal resistance of defective graphene was investigated [13,14]. They have considered constrictions constructed by linear vacancy defects (very thin rectangular defects) and demonstrated that the thermal resistance is a decreasing function of the width of the constrictions and is independent of the heat current. It has been reported that the ballistic thermal resistance of graphene nano-junctions is independent of the length and convex angle but it is inversely proportional to the constriction width [15]. However, increasing the thermal resistance has an adverse effect on heat dissipation; and this

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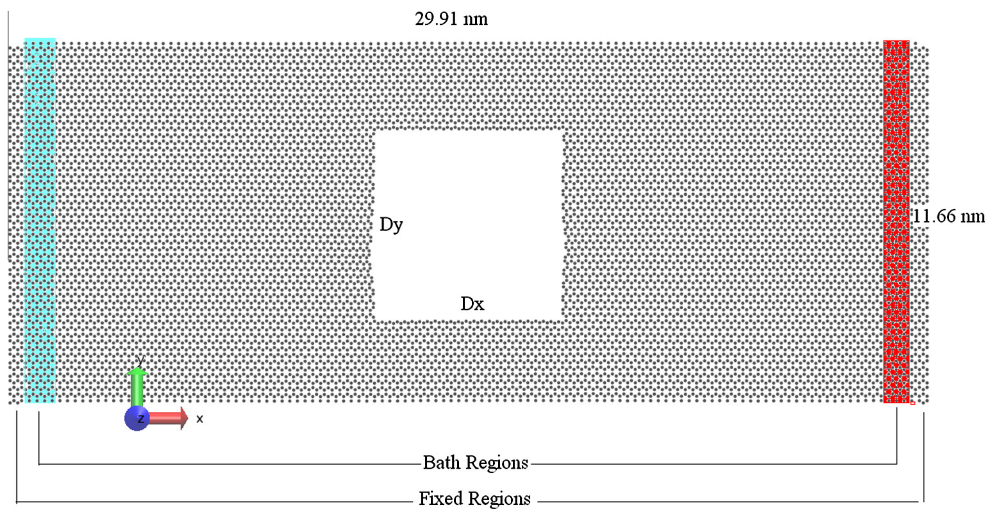

Fig. 1. Snapshot of the schematic representation of the atomic structure of system.

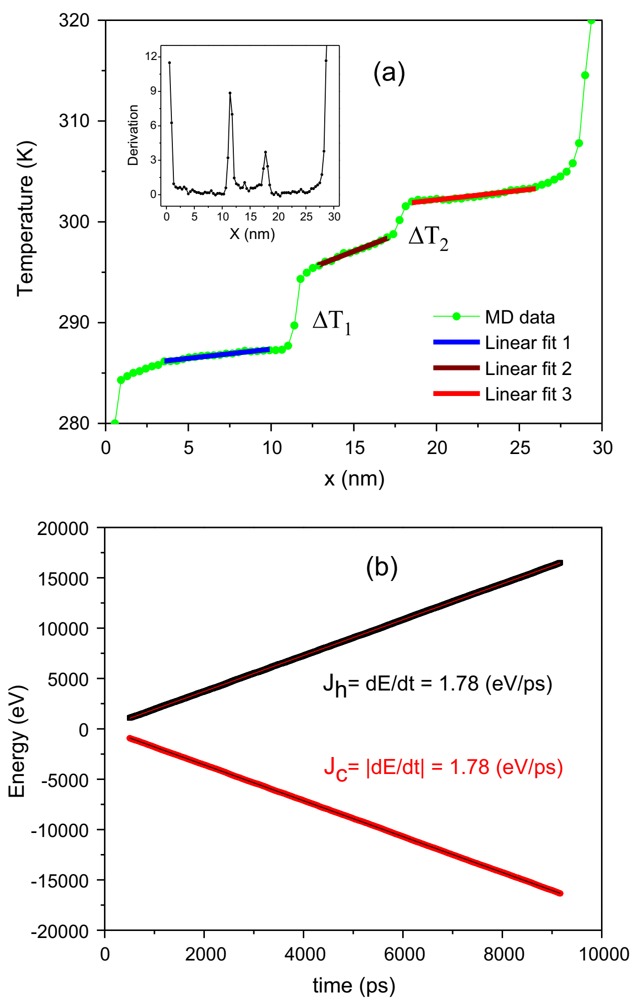

Fig. 2. (a) A typical temperature profile for defective graphene (square defect with 6 nm in size). The inset shows derivation of profile to distinguish jump points. (b) Energy added to the hot bath (black) and subtracted from the cold bath (red) versus time. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

phenomenon can be utilized to enhance the figure-of-merit in thermoelectric applications [16].

Therefore, from a practical point of view, understanding the effect of defect on thermal transport properties is important in designing nanostructured thermoelectric materials and thermal management. It is plausible that, purposeful engineering of defects can be utilized to accurately tune the thermal properties of graphene.

The goal of the present paper is to compute the thermal resistance of a rectangular defective graphene and its dependence on the width and height of the defect using molecular dynamics (MD) simulation method [17]. The paper is organized as follows. In Section 2, the computational methodology and the simulation details are provided. Section 3 reports on the simulation results and discussion. Finally, concluding remarks of our study are summarized in Section 4.

2. Computational methodology and simulation details

Here, we used non-equilibrium molecular dynamics simulation technique [6,18] to compute the thermal transport. All simulations were performed using the LAMMPS software package [19,20]. The optimized Tersoff potential was used to model the carbon-carbon covalent bonding interactions of graphene atoms due to its accurate handling of phonon dispersion [21]. Equations of motion were integrated via the velocity Verlet algorithm [17] with a time-step of 0.5 fs. The total length of the system was set at 29.91 nm and the width was set at 11.66 nm. Fixed boundary conditions were employed along the heat flow direction (x-direction) to prevent translation and rotation of the system. Periodic boundary conditions were used perpendicular to heat flow direction (y-direction), and the out-of-plane dimension of graphene was kept sufficiently large. Nose-Hoover thermostat [22,23] was applied to maintain the system at a constant temperature. First, each structure was equilibrated for 0.5 ns (1million time steps) within the constant-(NVT) ensemble, and the temperature was set at $T_0 = 300$ K. Then, the global thermostat was switched off and we applied two hot and cold heat baths, whose temperatures were $T_0 + \Delta$ and $T_0 - \Delta$, respectively. In order to avoid any artificial effects, all the simulations were carried out with the same thermostat parameters and Δ was set at 20 K. Each simulation was continued for 0.5 ns to reach a non-equilibrium steady state, and then for 5 ns to average the temperature profile over time. The system was equally divided into 80 slabs along the x direction and the local temperature for each slab T_{MD}, was calculated from the kinetic energy of atoms according to the Boltzmann distribution