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Thermal rectification in partially hydrogenated graphene with grain boundary, a non-equilibrium molecular dynamics study

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ABSTRACT

In the present study, we have tried to investigate thermal conductivity and thermal rectification in the partially hydrogenated graphene sheet with grain boundary through non-equilibrium molecular dynamics simulation method. To this end, the 3-body Tersoff and the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential were employed. The results revealed that the grain boundary plays an important role in phonon scattering, which flows to the other side of grain boundary. It was observed that temperature drops significantly across a grain boundary that leads to the thermal resistance. It has been also proved that thermal rectification depends on the temperature difference between two ends of the system. Also in such a system, a tuning factor for the tuning of the thermal rectification has been introduced by randomly removing hydrogen atoms of the partially hydrogenated graphene sheet with grain boundary.

1. Introduction

Graphene is a nano-sized molecule of carbon atoms in the form of a two-dimensional honeycomb lattice structure, in which carbon atoms have sp2 covalent bonds [1,2]. Much attention has been paid to the unique properties of graphene such as mechanical [2–7], electronic [8–12] and thermal [13–21] properties in the past decade. In order to develop silicon-based micro-sized devices, we need to search for a new type of material with high thermal conductivity to manage and control the heat of the system. Due to its high thermal conductivity, graphene is an appropriate candidate to the thermal transport and heat management among nanoscale materials [22]. Another application of thermal conductivity of graphene is to generate a driving force to move molecules, utilizing the temperature gradient [23,24]. Shahil and others [15] have reviewed its thermal properties, heat management and the applications of graphene, as well as multilayer graphene of advanced electronics and optoelectronics. Several investigations have been conducted about thermal transport and thermal conductivity of graphene-based composites [25–28]. To modify thermal conductivity of polymers (which is about 0.1–1 $W\,m^{-1}\,K^{-1}$) up to higher values, graphene is added to it [29]. Moreover, the graphene wrinkle (GW) is a novel molecule that its thermal conductivity was investigated [30]. The GW shows relatively low thermal conductivity than that of pristine graphene. To manage heat conduction in the micro-electronic devices, telescopic silicon nanowire has been also suggested [31]. In the telescopic geometry of silicon nanowire, the thermal rectification was calculated by non-equilibrium molecular dynamics simulation (NEMD), and theoretically was studied for various temperature differences between two ends of nanowire. The thermal rectification indicates that there is a priority in direction for heat flow. Therefore, thermal conduction in one direction is greatly compared to the opposite one. Among the carbon-based nanostructures, Hydrogenated graphene (graphane), which assumes hydrogen atoms attached to both sides, has also remarkable thermal conductivity [32]. In the graphane, sp2 bond between carbon atoms transforms into sp3. All properties of graphene can be controlled through hydrogenation of graphene [33]. Therefore, the graphene and graphane open numerous properties, making it possible to use them for nanoscale thermal management. Recently, Ali Rajabpour and others [34] have investigated thermal transport in graphene-graphane nanoribbon or patterned hydrogen functionalized graphene, using NEMD simulation and consequently have found a thermal resistance at the interface of graphene-graphane. The thermal resistance can make this setup as the thermal rectifier with remarkable performance. In the structure discussed in [34] the interface includes no defect, and all rings are hexagonal in the interface and also direction of two sides is the armchair. Another system which is similar to graphene-graphane, that was discussed above, has been introduced by Yazyev and Louie, LAGBI [35]. LAGBI is a graphene with a grain boundary. A

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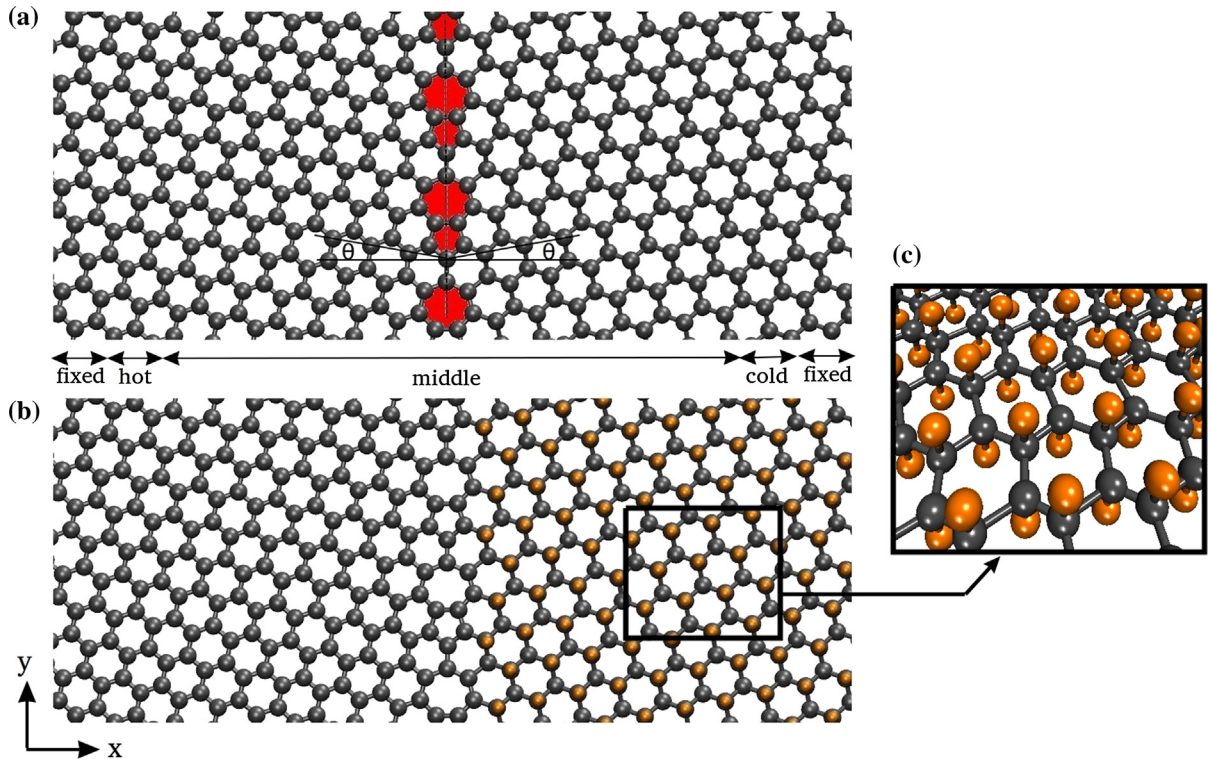

Fig. 1. (a) Atomic structure of the model which shows two misorientation graphene connected via grain boundary (colored by red) with $2\theta = 32.2^\circ$ (LAGBI) and, (b) the full hydrogenated of right side of LAGBI (F-LAGBI), (c) cross-section view of selected portion. Carbon and hydrogen atoms are colored by gray and orange, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

grain boundary is introduced as an array of pentagon-heptagon defects along the y direction that its misorientation angle of two sides is $2\theta = 32.2^\circ$ (see Fig. 1(a)). Lotfi and Neek-Amal [21] have studied temperature profile in LAGBI and revealed that there is a thermal resistance at the grain boundary. The observed temperature gap in grain boundary is 10 K while temperature difference was 20 K and the length of sheet was 30 nm.

In the present work, we have intended to investigate the thermal conductivity of both sides of LAGBI nanoribbon and thermal rectification of patterned hydrogen functionalized LAGBI nanoribbon. The patterned hydrogen functionalized LAGBI, will be introduced as an appropriate apparatus for the thermal rectifier.

2. Computational method

In this study, all of simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [36,37], which is a classical molecular dynamic code. In this stage, a system of graphene sheet with dimensions 20 nm × 10 nm containing a grain boundary with misorientation angle $2\theta = 32.2^\circ$ (LAGBI) which has already been introduced in the [38] is considered, and also the right side of grain boundary is assumed to be full hydrogenated (F-LAGBI) the same as graphane, which is a form of hydrogenated graphene in both sides in an alternating manner. In fact, the grain boundary is the interface between domains of graphene with different crystallographic orientation. Moreover, to generate partially hydrogenated of right side of LAGBI, we randomly removed H atoms from the both sides of F-LAGBI (P-LAGBI). In the F-LAGBI and P-LAGBI there is no symmetry, so that they can be an appropriate candidate for thermal rectifier. In order to model interactions between C—C and C—H atoms in the system, we considered AIREBO potential [39]. The Motion equation is integrated with time step 1 fs, by velocity Verlet algorithm. Also, we have applied free boundary condition to all directions. First, whole of the system was coupled with the NVE ensemble, as well as Langevin thermostat [40] to reach thermal equilibrium for 500 ps. Then, to calculate the local temperature on the sheet, it was divided to regions with 1 nm width. So, two end regions, as illustrated in Fig. 1(a), were fixed during simulation time. Two other regions which have been specified as cold and hot regions are coupled with Nose-Hoover thermostat [41,42] to generate the temperature gradient across the sheet and also steady-state heat current for about 500 ps simulation time. The hot and the cold regions' temperature were set to $T + \Delta$ and $T - \Delta$, respectively, where T and 2Δ are the mean temperature of system and the temperature difference between the hot and the cold regions, respectively. The NVE ensemble was applied between the hot and the cold regions (middle region). After reaching to steady state, the heat flux was calculated as energy per time unit per area that is extracted from the hot region and enters to the cold region. The heat flux and the regions' temperatures were averaged over 500 ps and presented as the results. To obtain thermal conductivity, we used Fourier's law $j = -\kappa \nabla T$. Prior to rectification calculations, thermal conductivity $\kappa(T)$ for both graphene and graphane sheets was obtained with the same orientation as those domains in F-LAGBI. The sizes of sheets were considered 10 nm × 10 nm. The thermal rectification is then calculated for F-LAGBI and P-LAGBI.

3. Results and discussions

The non-equilibrium molecular dynamics simulations were carried out to obtain thermal conductivity and thermal rectification graphene-based nanostructures. As depicted in Fig. 2, thermal conductivity of graphane was obtained with the same orientation, which is approximately equal to half of graphene, that is due to the conversion of sp2 bondings in graphene to sp3 one's in graphane