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Molecular dynamics study of temperature behavior in a graphene nanoribbon

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ABSTRACT

Unlike an independent variable in classical continuum mechanics, temperature at molecular dynamics simulation is perceived as a spatiotemporal averaged quantity from the velocity field of atoms in system of interest. Following this definition, an intriguing correlation between displacement and temperature in graphene nanoribbon under impulsive loading has been captured at the early stage of simulation to demonstrate that temperature variation along a specific direction behaves like a wave motion, while at the end of simulation temperature field reaches to a steady state like a classical diffusion equation of temperature. This riveting phenomenon offers insights into the thermal–mechanical coupling phenomena of nanodevices.

1. Introduction

Does the temperature variation along a specific direction behave like a wave motion? From the viewpoint of classic heat conduction theory, the answer is no since it lacks the foundation to interpret the wave-like energy transport phenomenon, 'second sound' [1]. However, this unprecedented phenomenon has been observed in superfluid [2,3] and pure crystals [4] at cryogenic temperatures. To capture the unconventional property and tackle the challenge posted by the classical theory, Green and Naghdi [5] proposed a promising non-classical theory followed and extended by Jordan and Straughan [6], Bargmann and Steinmann [7], based on the concept of artificially incorporating a scalar history variable, thermal displacement, as the time interval over the empirical temperature. The fundamental physical meaning of the thermal displacement in the Green-Naghdi theory, however, remains elusive and debatable. On the other hand, from the molecular dynamics simulation perspective, temperature is a measure of the instantaneous kinetic energy in a system [8], which is perceived as a dependent variable, a spatiotemporal averaged quantity from the velocity field of atoms in system of interest unlike being an independent variable governed by the conservation of energy in classical continuum mechanics. The definition of temperature at nanoscale may offer a feasible way to reproduce the intriguing wave-like behavior of temperature variation along a specific direction. Meanwhile, graphene nanoribbon has gained the appreciable popularity in a variety of applications due to its outstanding architecture and properties [9–16]. Therefore, following the definition of temperature at MD simulation, we investigate the temperature variations of graphene nanoribbon under an impulsive mechanical loading to see if there exists the wave behavior of temperature profile along a specific direction at nanoscale.

2. Simulation method

Molecular dynamics simulations package developed by the author and visualization program VMD are employed to perform the simulations and analyses with Tersoff force field [17]. Tersoff potential has been perceived as one of the well-accepted and proven 3-body potential to give a quantitatively accurate description of the pairwise and many-body interactions in the graphene sheet. To exclude the unphysical high bond force arising from improper cutoff functions, we set the cutoff as 2.5 Å, and there is no periodic boundary condition in the three directions. Meanwhile, to rule out noise effects due to edge effects and make the correlations between wave propagation and temperature variation more pronounced, the system takes a long period of relaxation to dissipate the deleterious side-effects. Nosé-Hoover thermostat [18] has been employed to control the reference temperature of the system before applying any kind of boundary conditions.

A pristine graphene nanoribbon with length 43.2 nm and width 2.1 nm is constructed in Figure 1. To better illustrate the temperature variation during the simulation process, Region 2 of the graphene nanoribbon as depicted in Figure 1 is equally partitioned along the z-axis into 20 subgroups with around 170 atoms for calculating the local temperature while Region 1 is designed as boundary condition for input signal and Region 3 is fixed. The input signal is a half-sine impulsive loading with magnitude 2.0 nm and duration 1 ps along the z-axis direction. The NVT ensemble is used to control the reference temperature of the whole system before applying any boundary conditions. NVT is applied to all atoms in the systems for initiating a reference temperature for 0 K and 300 K,

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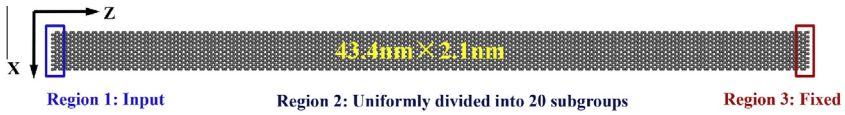

Figure 1. Computational model of graphene nanoribbon.

respectively. After the equilibrium state is achieved, NVE ensemble simulations are carried out to control the Region II in the specimen. The atoms in Region I and III are considered to NVT but with fixed position after the impulsive loading. There is no periodic boundary condition in MD simulation. The total simulation time is 28.83 ps after relaxation and equilibration.

3. Results and discussion

Here, we adopt a popular definition of temperature in the MD simulations [8], as a space-averaged variable of a group of atoms, $T(t) = \frac{\sum_{i=1}^{N} m_i[\mathbf{v}_i(t)-\bar{\mathbf{v}}]^2}{3k_B N}$, where N is the number of the group of atoms; m_i the mass of atom i; $\mathbf{v}_i$ the velocity of atom i; $\bar{\mathbf{v}}$ is the average velocity of the group of atoms; k_B the Boltzmann constant.

Figure 2 presents the snapshots of the deformed graphene nanoribbon with the temperature profile as simulation time. The blue and red color represents the minimum and maximum value of temperature in the system, respectively. It is clearly observed that the crest of mechanical wave engendered by the input impulsive loading propagates into the graphene nanoribbon along the z-axis direction just like ocean wave. The magnitude of the crest in mechanical wave is close to but less than that of input impulsive loading at the early stage of simulation as depicted in Figure 3, indicating that a fraction of the translational kinetic energy of the system has been converted to the internal vibration of graphene nanoribbon, notably in the temperature mode. It is apparently noticed in Figure 2 that, with time proceeding, the region with maximum value of temperature along z-axis direction propagates along with the mechanical wave, thereby offering clues that temperature variation along the z-axis behaves like a mechanical wave at the early stage of simulation. Also the speed of temperature variation explicitly calculated from the simulation results is around 3.72 km/s, which is far below the ideal sound wave speed of graphene ribbon, 21.7 km/s [19], provided that the graphene ribbon are assumed to be an ideal continuum solid.

To better illustrate the intriguing point, Figure 4 provides a quantitative analysis of energy transmission related to velocity field by showing the temperature variation profile along the z-axis direction at different simulation time. The temperature values in Figure 4 represent the subgroup calculations not a finite x-coordinate. It is clearly depicted that at the early stage of simulation, for example, t = 0.24 ps, there is only one subdivision in the specimen possessing high temperature while others keep temperature around 0 K. As time goes on until t = 8.55 ps, the peak of temperature profile moves into the specimen with almost the same magnitude while temperature of the rest part in the graphene nanoribbon keep close to 0 K but not 0 K. This can be elucidated by the fact that the nonlocality and nonlinearity of the interatomic forces trigger the vibrations of atoms far from the reaction field, which eventually produces the temperature variation of the system. At t = 28.83 ps, the temperature variation of the whole system excluding the peak effect reaches to a steady state with temperature 550 K which captures the distinct feature of diffusion equations of temperature in classical continuum mechanics. This can be attributed to the fact that once the energy associated with the mechanical wave is converted into internal energy it tends more to spread out over the entire domain rather than convert back again. In order to study the effect of reference temperature of the system on the thermal impulse, Figure 5 presents the snapshots of the deformed graphene nanoribbon with the temperature profile as simulation time at the reference temperature 300 K, and Figure 6 provides a similar quantitative analysis of energy transmission related to velocity field at the reference temperature 300 K as we did in Figure 3. Differences between these two sets of result can be attributed to the thermal noises from the varying reference temperature. The key characteristics of thermal impulse in two sets of simulations remains pronounced. To summarize, Figure 4 provides significant insight to offer a panorama of the peculiar temperature variation behavior along the z-axis direction in the molecular dynamics simulation, which will pave the way to better understand the fundamental physical meaning and properties of temperature at nanoscale.

As depicted in the previous content, Figures 3(a–d) exhibit the correlation between the displacement profile and temperature variation profile of specific subgroups along the z-axis direction in the systems as simulation time. By comparison, it is clearly observed that the motion of the temperature peak along the z-axis direction unanimously coincides the wave crest front at the early stage of simulation while after a long period of time the temperature of

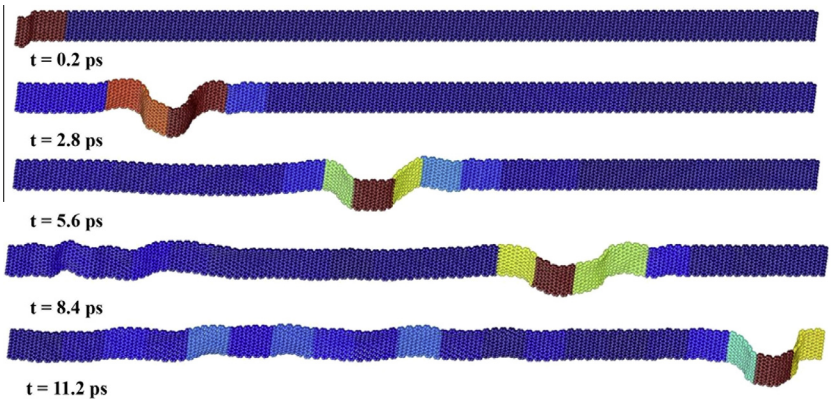

Figure 2. Evolution of temperature variations at atomic arrangement as simulation time. Dark red color represents the maximum value of temperature region in the snapshot under reference temperature 0 K. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)