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A molecular dynamics based investigation of thermally vibrating graphene under different boundary conditions

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HIGHLIGHTS

- This work investigates combined effect of length scale, temperature and boundary conditions on characterizing ripples in graphene.
- The freely vibrating edges have a prominent contribution in determining the shape and vibrational modes of the ripples.
- With increasing length scale the natural frequency of vibration decreases and the amplitude of the ripples increases.

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ABSTRACT

In this paper we have investigated the ripples in graphenes under thermal agitation. It is known that as temperature increases ripples originate in the flat landscape of a graphene sheet which is responsible for changing its properties. Among a limited number of works available in literature the role of length scales and temperature on the characteristics of the ripples has been investigated. However it is important to include the boundary conditions with other parameters in order to get a broader picture. In this work graphenes with three different sizes (2 nm, 10 nm and 50 nm) were considered under both *simply supported* and *free-opposite-sides* boundary conditions at different temperatures (e.g. 10 K, 100 K and 500 K) using molecular dynamics simulations. The variation in natural frequencies and their dependency on the boundary condition, length scale and temperature was thoroughly studied. Change in the boundary condition can introduce new modes of vibrations in graphenes. A combined effect of length scale, boundary condition and temperature was shown to be responsible for developing the geometrical patterns in the ripples. With free-opposite-sides boundary conditions the ripples are more harmonic in larger graphene than other cases. It was also noticed that the probability distribution for the off-plane displacements of the carbon atoms in graphene is typically non-stationary at small length scales. Variation in boundary conditions and length scales may affect the kurtosis of the distribution. The results showed adequate agreement with available data in the literature.

1. Introduction

Graphene is a 2*D* carbon based nanomaterial which has drawn a significant amount of attention from the scientific community in last few years. The sp^2 bonded carbon atoms in the graphene exhibit almost similar behavior compared to other carbon based nano materials such as "Carbon nanotubes (CNTs)" [1]. Graphene has a wide range of applications due to its outstanding electrical, mechanical and thermal properties [2]. Although graphene is a 2*D* crystalline material, at finite temperature it has a tendency to be crumpled up. This introduces ripples in a graphene sheet. Existence of multiple ripples may change the nonlocal interaction among the carbon atoms in graphene as well the crystallinity. The wavelength of the ripples in graphene is very important in determining the long-range interaction among the atoms in the graphene [3]. These ripples exhibit non-stationary behavior and introduces different modes of vibrations at different temperatures. So it is an interesting feature for graphene which needs proper attention. There are not too many works available in the literature along this direction. Hsieh and co-workers studied the effect of temperature on degrading the mechanical properties of CNTs [4]. Using the nonlocal plate theory Shen and co-researchers investigated the role of temperature on the properties of simply supported graphenes [5]. Besides mechanical properties ripples in

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Table 1
Summary of the graphene sheets.

System	$L_x = L_y$	Number of atoms
Type-a	2 nm	180
Type-b	10 nm	4798
Type-c	50 nm	96,288

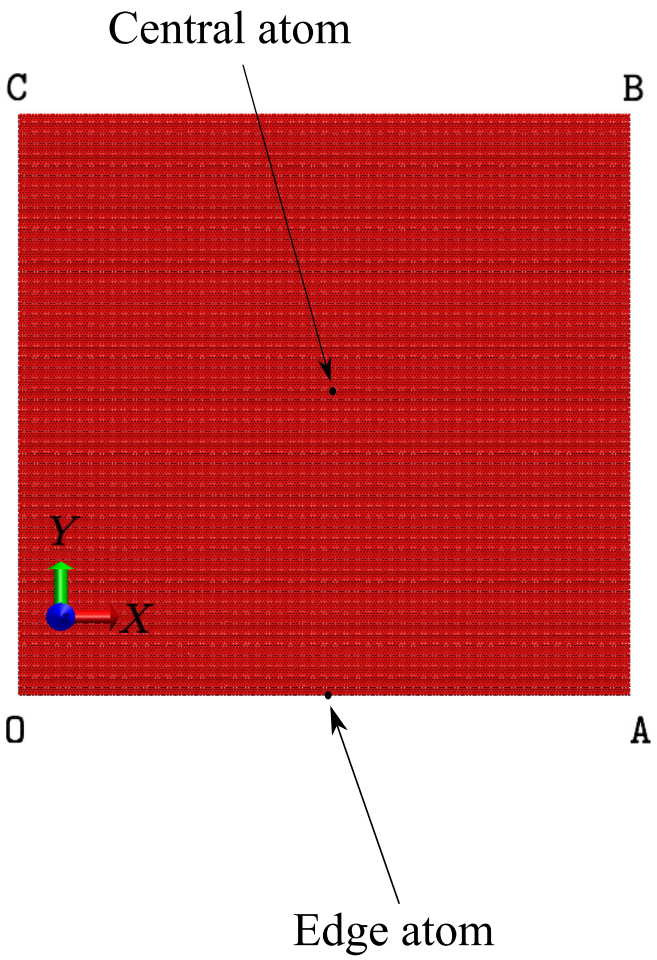

Fig. 1. A 50 nm × 50 nm graphene sheet.

the graphene lead to inhomogeneous charge distribution too [6]. The expected mechanical or electrical properties of a "flat" graphene may not be present in real-life applications. Even at room temperature graphene of certain length scale has a tendency to be crumpled up. Ripples can be formed due to many reasons. Thermal vibration, axial compression [7], interfacial mismatch between graphene and substrate [8] etc., are few well-known reasons. In the current work the interest is limited to freely vibrating graphene under thermal influence. The behavior and propagation of ripples under the given condition still demand for further investigation. Besides variation in length scale and temperature, boundary conditions play a significant role on the mechanism of ripples. A combined effect of length scale, temperature and boundary condition is thoroughly studied in this paper. The nature of ripples in graphene was initially investigated by Smolyanitsky and Tewary by using classical molecular dynamics (MD) simulation [9]. They showed the nature of ripples in a graphene with $L_x = 13.6$ nm, $L_y = 15.8$ nm considering external force and finite temperature under simply supported boundary condition. In another work RuMeng and LiFeng [10] studied the vibration of single layered graphene considering different temperatures and length scales. They compared the result from MD with the classical plate theory under simply supported and two opposite sides free boundary conditions. In another work by Fasolino and co-researchers the random ripples were investigated at different length scales and temperatures [3]. A thorough investigation on the nature of ripples and their dependency on length scales as well as boundary conditions are still very much unexplored by the researchers. So it has been an intriguing matter among the researchers to investigate the effect of length scale as well as different boundary conditions on the nature of ripples in the graphene at different temperatures. In addition to that the displacements at two crucial locations (i.e. center and free edge of the graphene) and the non-stationary behavior of the displacement filed in terms of histogram/probability need to be explored at different temperatures, length scales and boundary conditions. This can give us a clear insight on the nature of ripples. For a long period of time the ripples propagate back and forth between the free or fixed edges. It is important to investigate the pattern of these ripples and their long term nature pertaining to the role of boundary conditions. Works along the similar direction are seldom in the literature. In this work the nature of the ripples in graphenes under different boundary conditions is studied using classical molecular dynamics (MD) simulation. The role of both high and low temperatures and different length scales are incorporated in the investigation. Current work was able to perform an in-depth investigation on the nature of ripples under different circumstances and compare specific results corresponding to specific cases available in the literature.

2. Computational details

2.1. Development of graphene sheets

In this work graphenes with three different dimensions are considered. These are named as Type-a, Type-b and Type-c graphenes based on their lengths: 2 nm, 10 nm and 50 nm, respectively. The details are given in Table 1. In Fig. 1 Type-c graphene is shown. The sides OA, CB are parallel to X axis and OC, AB are parallel to Y axis. Two different types of boundary conditions (BC) are used: BC_1, BC_2. In BC_1 two opposite sides OC and AB are constrained. The other two opposite edges OA and CB are free. All the edges are constrained to move in X, Y and Z directions in BC_2. It will be seen that the boundary conditions play a vital role in the thermal vibration of graphene.

From the point of view of applications as a membrane BC_2 is more typically used than BC_1. It is important to justify the motivation behind considering BC_1. The goal in the current work is to study the ripples and their correlation with the freely vibrating edges in a graphene under thermal influence. Thermal vibrations at nanoscale are merely random. So the freely vibrating edges may introduce some interesting features in the vibration of graphene sheets (discussed later). In addition to that there are several potential applications of graphene as sensors or electrodes where all four edges might not be fixed. Hence it is justified to study the nature of thermal ripples under both BC_1 and BC_2. The free edges can be chemically functionalized with different molecules which will be considered in future work.