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Energy exchange between vibration modes of a graphene nanoflake oscillator: Molecular dynamics study

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ABSTRACT

We investigated the oscillatory behaviors of a square graphene-nanoflake (GNF) on a rectangular GNF via classical molecular dynamics simulations, and analyzed the energy exchange and the oscillation frequencies for three different modes. The simulation results using a model structure show that the GNF oscillator can be considered as a high frequency oscillator. As its initial velocity increases, its telescoping region increases, then its structural asymmetry along the axis due to own small rotation exerted asymmetric van der Waals (vdW) force on it, and finally, this asymmetric vdW force enhances its rotational motions during its axial translational motions. So the initial kinetic energy of the axial translational motion is changed into the energy of the orthogonal vibrational and the rotational motions. Its resonance frequencies are dependent on the aspect ratio of the bottom rectangular GNF, the difference between the lengths of the GNF oscillator and the bottom rectangular GNF, and the initial velocity.

1. Introduction

Nanostructured materials have gained great importance in the past decade on account of their wide range of potential applications in many areas [1]. Especially, nanoelectromechanical systems (NEMSs) are drawing interest from both technical and scientific communities [2]. Since their discovery in 1991 [3], carbon nanotubes (CNTs) have attracted enormous attention for their fundamental behavior and for their use in a wide variety of applications in nanoelectronic devices [4–6], probe tips for scanning probe microscopes [7–11] or in the automotive and aerospace industries for the dissipation of electrostatic charges [12,13]. Gigahertz CNT-based oscillators were proposed by Zheng and Jiang [14] after Cumings and Zettl [15] reported an ideal low-friction and low-wear bearing carved out of a multi-walled CNT with a diameter of a few tens of nanometers. Ultra-fast CNT oscillators have been intensively investigated, and they are expected to be applied to nanoscale sensors, actuators, resonators, injectors, motors, engines, filters, memories and switching devices [16].

When fabricated as mechanical components of nano-machines, the properties of friction and energy dissipation are extremely important since they can severely affect the performance and energy consumption of the devices [17,18]. Hence, the super lubricity of graphite has been investigated [17,18]. Recently graphene [19–21] has also been highlighted as an ideal lubricant for micro-electromechanical systems (MEMSs) and nanoelectromechanical systems (NEMSs) [22,23], for which traditional lubricants can no longer function normally [24]. In 2008, Zheng et al. [25] reported a self-retracting motion of square graphite-nanoflakes (GNFs) sheared from SiO_2-covered graphite islands and discussed the potential applications in NEMSs with a wide range of mechanical frequencies from megahertz and gigahertz.

However, square GNFs, which have been considered in the previous works [25–30], have a great drawback in their application to a stable oscillator because the translational motion of the square GNF rapidly transforms into its rotational motion [29,30]. Therefore, for GNFs, when this transformation from the translational to the rotational motions can be restricted, these GNFs have a great potential application in high-frequency oscillators. So, in this work, we consider long rectangle GNFs instead of square GNFs, as shown in Fig. 1, which shows the model schematics for a square GNF oscillator on a long rectangular GNF. The structural difference between its length and width of the long rectangle GNF hinders the kinetic energy transformation of the square GNF from the translational to the rotational motions during it oscillation. Basic three planar oscillation modes of the square GNF on the long

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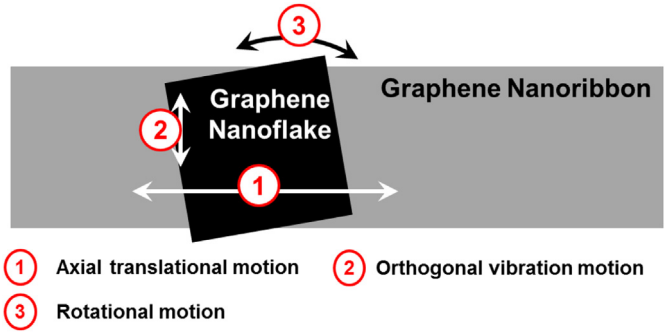

Fig. 1. Simple model schematics for a square GNF oscillator on a long rectangular GNF.

rectangle GNF are displayed in Fig. 1. In this work, we investigate the oscillatory behaviors of a square GNF on a long rectangle GNFs by using classical molecular dynamics (MD) simulations and analyze the oscillation frequencies for three different modes. Our results present that such a model graphene structure can be considered as a high frequency oscillator.

2. MD simulation methods

To investigate the GNF oscillator, we perform classical MD simulations, using a nanostructure, which is composed of the square-like GNF of 166 atoms (1.97 nm × 1.99 nm) on a rectangular GNF of 650 atoms (7.9 nm × 1.99 nm). The aspect ratio of the rectangular GNF is about 4. We used an in-house MD code that has been used in our previous studies [31–37] via the velocity Verlet algorithm, a Gunsteren–Berendsen thermostat to control the temperature, and neighbor lists to improve the computing performance. The MD time step was 5×10^{-4} ps. We assigned the initial atomic velocities to a Maxwell distribution, and the magnitudes were adjusted in order to fit the temperature of the system. Interactions between carbon atoms that form the covalent bonds of graphene were described using the Tersoff–Brenner potential [38,39]. The long range interactions of carbon were characterized according to the Lennard–Jones 12–6 (LJ12–6) potential with the parameters that were given by Mao et al. [40]. In this paper, the parameters of the LJ12–6 potential were $\varepsilon = 0.0042$ eV and

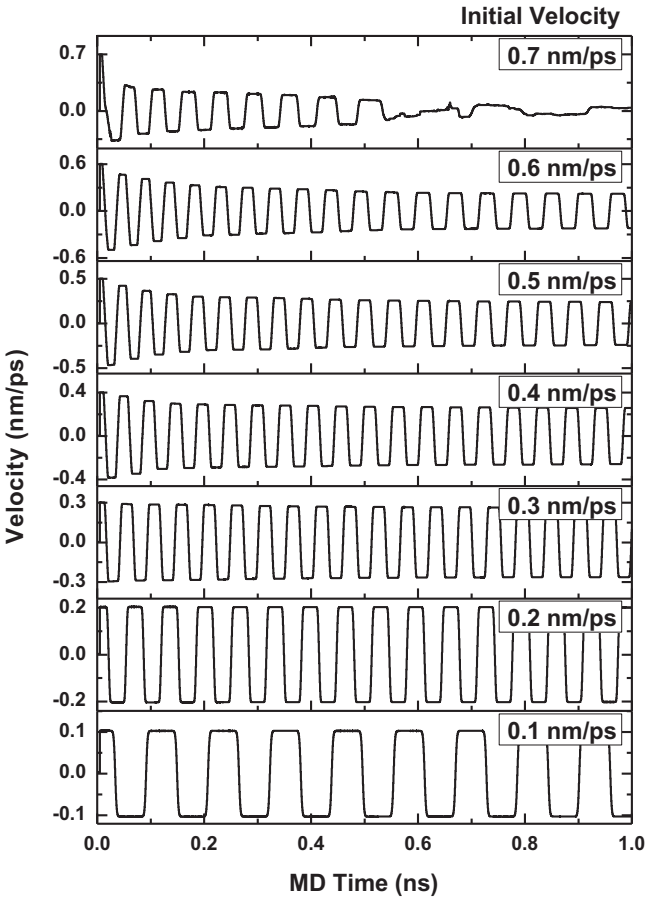

Fig. 3. Velocity variations of the GNF oscillator in the direction of the axis as a function of the MD time for seven different v_0.

$\sigma = 3.37$ Å. The cutoff distance of the LJ12-6 potential was 20 Å. Initially, the GNF on GNR was relaxed without an external force. For all MD simulations, the temperature was set to 1 K and the rectangle GNF as the top layer of the patterned graphite was fixed. During the initial 5 ps, the GNF freely moved without external

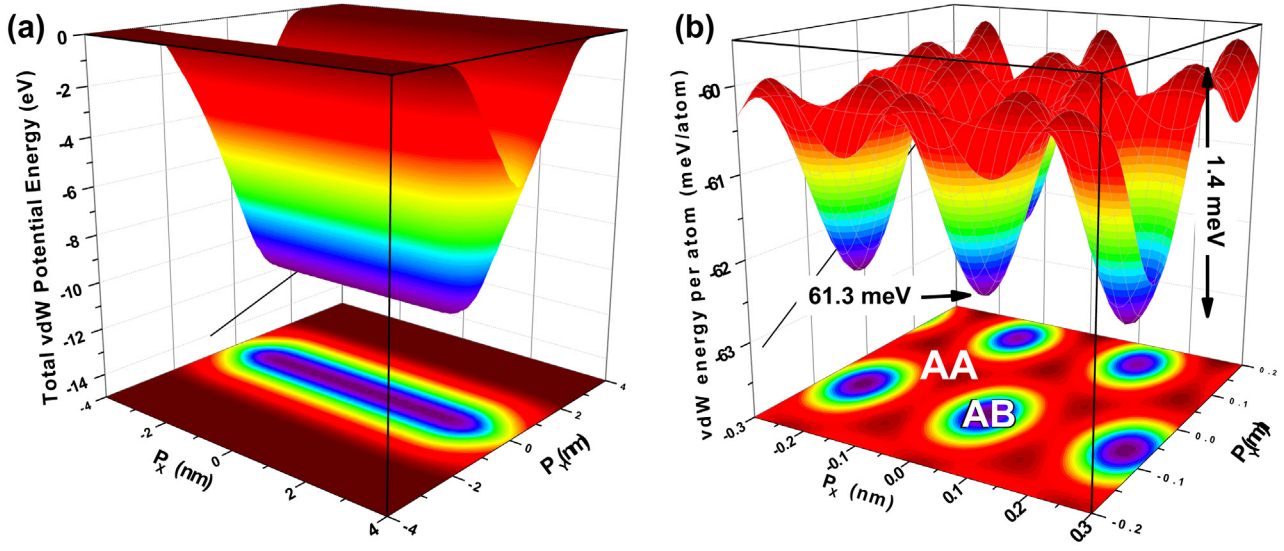

Fig. 2. (a) Interlayer energy between the GNFs as a function of the in-plain relative displacement of the GNF oscillator when the interlayer gap was kept at 0.335 nm. (b) Interlayer energy per atom of the GNF oscillator versus in-plain relative displacements.