

Molecular Dynamics Simulation Study on Nanoelectromechanical Oscillator based on Graphene Nanoflake

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ABSTRACT

Recently graphene has also been highlighted as an ideal lubricant for microelectromechanical systems (MEMSs) and nanoelectromechanical systems (NEMSs), where ‘traditional’ lubricants no longer function normally. Atomic-scale graphene can be fabricated using micro-mechanical chop crack, thermal expansion, and extension growth techniques. Monolayer graphene is considered a suitable material for investigating two-dimensional quantization phenomena, such as temperature-trigger plasma, quantization absorption spectrum, and the fractional quantum Hall effect. Additionally, the hexagonal symmetric structure of graphene makes it a candidate material for nano devices. Here, we investigated the translational and rotational motions of a square graphene nanoflake with retracting motions by performing classical molecular dynamics simulations. Our results show that the kinetic energy of the translational motion was exchanged into the kinetic energy of the rotational motion. Thus, square graphene nanoflake oscillators have very low quality factors in translational motions. We discuss that square graphene nanoflakes have great potential to be a core component in nanoelectromechanical systems by detecting their motions with ultrahigh sensitivity to facilitate the development of sensor, memory, and quantum computing.

Keywords: Graphene Flake, Molecular Dynamics, Graphene Oscillator

1 INTRODUCTION

Nanostructured materials have gained great importance in the past decade because of their wide range of potential applications in many areas.[1] In particular, nanoelectromechanical systems (NEMSs) are attracting interest from both the technical and scientific communities.[2] When used as mechanical components of nano-machines, the properties of friction and energy dissipation are important because they can greatly affect the performance and energy consumption of the devices.[3,4] For carbon nanotubes (CNTs),[5] as a nanomaterial with low friction between interlayers, Zheng and Jiang[6] proposed gigahertz CNT-based oscillators after the report of Cumings and Zettl,[7] which addressed an ideal low-friction and low-wear bearing carved out of a multi-wall CNT with a diameter of a few tens of nanometers. Since

then, CNT oscillators based on multi-walled CNTs have been investigated widely using MD simulations.[8-25]

“Superlubricity,” a regime of motion in which friction vanishes, or very nearly vanishes, is an important condition in achieving ideal NEMSs. Superlubricity can occur when two crystalline surfaces slide over each other in dry incommensurate contact. This effect, also called structural lubricity, was suggested in 1991 and verified with high accuracy between two graphite surfaces in 2004.[26] The atoms in graphite are oriented in a hexagonal manner and form an atomic hill-and-valley landscape, which looks like an egg crate. When the two graphite surfaces are in registry (every 60°), the friction force is high. When the two surfaces are rotated out of registry, the friction is largely reduced. This is like two egg-crates that can slide over each other more readily when they are “twisted” with respect to each other.

Observation of superlubricity in microscale graphite structures was reported in 2012 [4] by shearing a square graphite mesa a few micrometers across, and observing the self-retraction of the sheared layer. Such effects were also described theoretically for a model of graphene and nickel layers.[27] This observation, which is reproducible even under ambient conditions, shifted interest in superlubricity from a primarily academic topic, accessible only under highly idealized conditions, to one with practical implications for micro and nanomechanical devices.[28]

A state of ultralow friction can also be achieved when a sharp tip slides over a flat surface and the applied load is below a certain threshold. Such a “superlubric” threshold depends on the tip-surface interaction and the stiffness of the materials in contact, as described by the Tomlinson model.[29] The threshold can be increased significantly by exciting the sliding system at its resonance frequency, which suggests a practical way to limit wear in NEMSs.[30]

In this study, we investigated the energy exchange between vibration modes of a square nano-graphene-flake oscillator in superlubric and self-retracting motions via ‘classical’ molecular dynamics (MD) simulations. Computational simulation works have advanced this field and helped to reveal the potential of graphene devices in future technologies.

2 SIMULATION METHODS

To investigate the energy exchange between vibrational modes of a square nano-graphene-flake oscillator in superlubric and self-retracting motions, we perform

classical MD simulations using a tri-layered graphene flake (Fig. 1), composed of 510 atoms, $2 \text{ nm} \times 2 \text{ nm}$ in size. Initially, the graphene flake was relaxed with no external force. Optimal atomic configurations of the GNR under axial strain were obtained using a steepest descent (SD) method, which is the simplest of the gradient methods, from the atomic configurations of the GNR with a C-C bond length of 1.42 \AA and an inter-layer distance of 3.4 \AA .

Interactions between carbon atoms that form the covalent bonds of graphene were described using the Tersoff-Brenner potential. The long-range interactions of carbon were characterized according to the Lennard-Jones 12-6 (LJ12-6) potential with parameters provided by Mao et al. In this paper, the parameters of the LJ12-6 potential were $\epsilon = 0.0042 \text{ eV}$ and $\sigma = 3.37 \text{ \AA}$. The cutoff distance of the LJ12-6 potential was 10 \AA . We performed the classical MD simulations using in-house MD code that has been used in our previous works, using the velocity Verlet algorithm, a Gunsteren-Berendsen thermostat to control the temperature, and neighbor lists to improve computing performance. The MD time step was $5 \times 10^{-4} \text{ ps}$. We assigned the initial atomic velocities to a Maxwell distribution, and the magnitudes were adjusted to fit the temperature of the system. In all MD simulations, the temperature was set to 1 K . In MD simulations, the bottom and the top layers of the graphene flake were clamped and this condition was described as a fixed region on both layers. To actuate the graphene flake oscillator, initial velocities (v_{y0}) of $0.1\text{--}0.9 \text{ nm/ps}$ were applied to the core graphene nanoflake along the y direction.

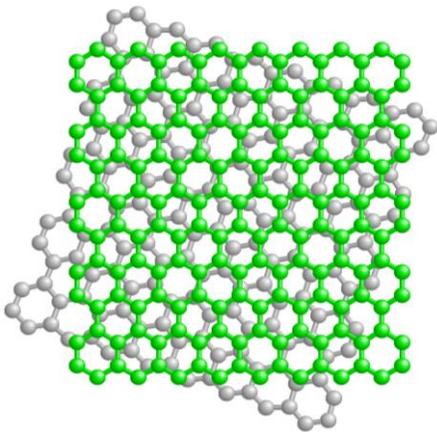


Figure 1: Tri-layered graphene flake, composed of 510 atoms, $2 \text{ nm} \times 2 \text{ nm}$ in size, for classical MD simulations.

3 RESULTS AND DISCUSSION

Figure 2 show the motion plots of the center and the edge of the core graphene nanoflake in the x - y plane for different values of v_{y0} . For the motion plots of the center, when the v_{y0} increased, the displacements in the y direction increased initially. However, for all cases, the one-

dimensional translational motions of the core graphene nanoflake along the y direction were rapidly damped during initial stage and finally its motions were converted into two-dimensional translational motions in the x - y plane. In Figure 2, we can also find the rotational motions of its edge. As the v_{y0} increased, the edge motions increased in the rotational motions. The kinetic energy of the initial translational motion was rapidly reduced, as discussed above, whereas the kinetic energy of the rotational motion increased; that is, the kinetic energy of the translational motion was exchanged into the kinetic energy of the rotational motion. Such a property indicates that because the graphene flake oscillators have very low quality factors in the translational motion, they have a weakness to become stable translational-motion oscillators.

To present the rotational motions of the core graphene flake, the relative rotational motions of the core graphene flake were calculated. Figure 2 shows the variations of the angle of an edge atom as a function of MD time for different values of v_{y0} . We can find the oscillations of the angle and their envelopes as signals.

The translational oscillatory behaviors of the graphene flake can be understood by the interlayer vdW energy and force variations, whereas the rotational oscillatory behaviors of the graphene flake can be understood by the transition of the core graphene flake into the incommensurate states. The pendulum-like motions found in some regions are closely related to the transition of the core graphene flake into the incommensurate states. Graphene layers can rotate relative to each other to incommensurate states in which the potential barriers of the interlayer interaction energy are smooth. At relative rotation angles $\varphi_0 = 0^\circ, 60^\circ,$ and 120° , graphene layers are commensurate and the potential energy barrier is significant to the relative motion of the layers.⁶⁸ However, when the layers are rotated relative to each other by an angle $\varphi_0 + \delta\varphi < \varphi < \delta\varphi - \varphi_0 + 60^\circ$ ($\delta\varphi \approx a_0 / L$, where a_0 is the lattice constant of graphene and L is the size of the layers), the layers become incommensurate and the barriers to the relative motion of the layers disappear. Such incommensurate states are observed in the form of so-called “Moiré patterns.” Although the transition of graphene layers to the incommensurate states has a considerable energy cost, it has been shown to play a significant role in static friction and thermally-activated diffusion of graphene flakes on graphene layers.

For translational motions, the oscillation dynamics of the graphene flake are similar to those of the CNT oscillators. However, there were significant differences in the potential reliefs of the interlayer interaction energy for graphene layers and carbon nanotube walls. Popov et al. discussed that the magnitude of corrugation of the potential energy relief was orders of magnitude higher for graphene layers than for nanotube walls. They examined the self-retracting motion of graphene flakes via MD simulations and analyzed the differences in the potential energy reliefs for graphene layers and nanotubes walls in

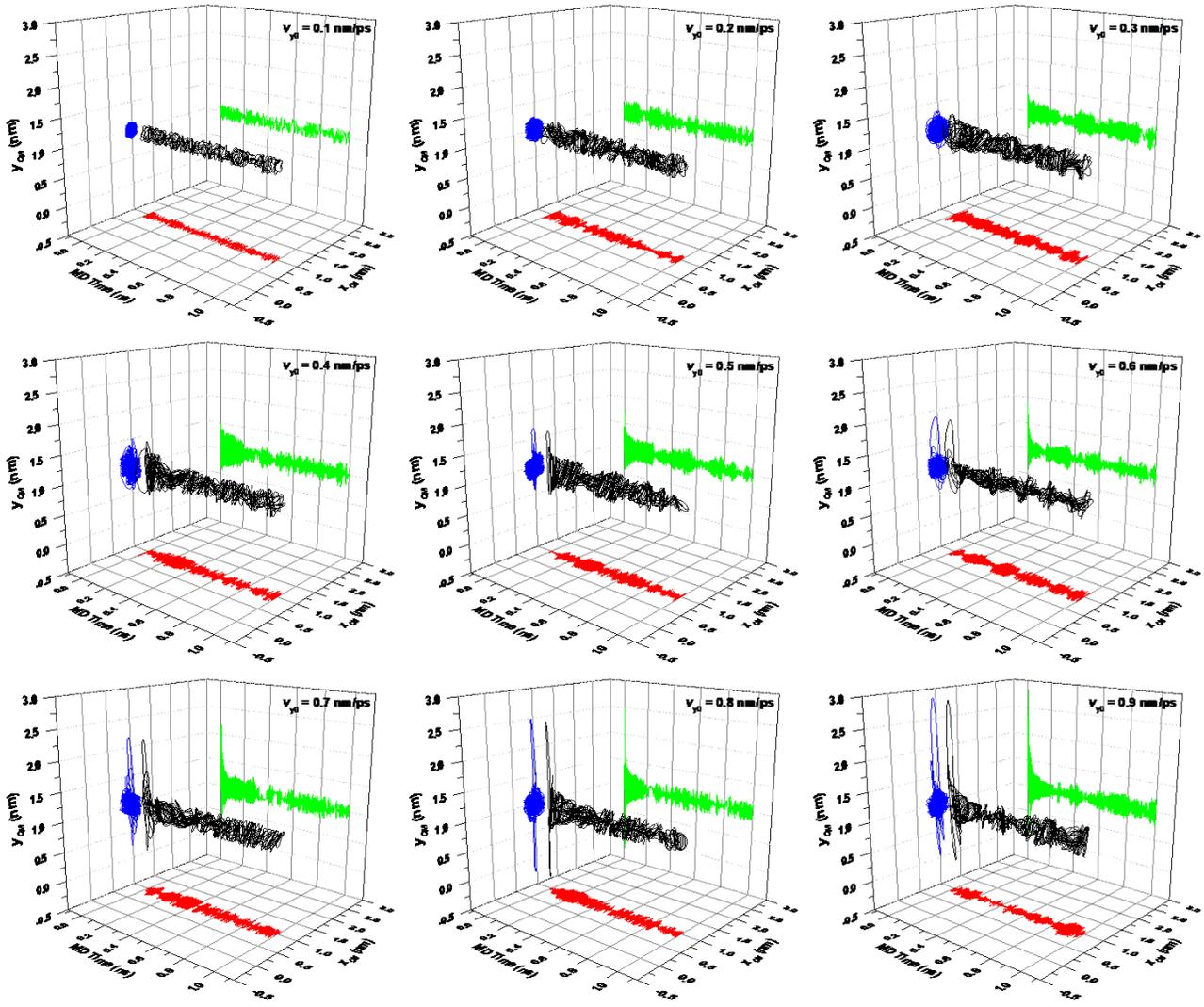


Figure 2: Motion plots of the center and the edge of the core graphene nanoflake on the x - y plane for different values of v_{y0} .

the essentially different dynamic behaviors. First, telescopic oscillations were suppressed for graphene flakes due to the excitation of flexural vibrations of the flakes. Second, the self-retracting translational motion of the extended flake was often accompanied by rotation of the flake. They investigated the influence of temperature, the direction of the telescopic extension, and the initial orientation and position of the extended flake on the possibility and characteristics of the self-retracting motion of the flake.

Generally, a graphene nanoflake oscillator with thousands of degrees of freedom can be reduced to a simple system with the few most relevant degrees of freedom in the presence of a thermal bath. We discuss the energy exchange mechanisms for the graphene nanoflake oscillator according to those for the graphene nanoflake oscillator addressed by Kwon et al. The few degrees of freedom

correspond to several important low-frequency mechanical modes, such as translational motion, orthogonal vibrational motion, and rotational motion, while the heat bath covers other higher frequency vibrations of the graphene nanoflake. When the kinetic energy leakage from the reduced system to the bath is slow enough, an energy exchange takes place between the translational motion and the orthogonal vibrational and rotational motions.

The MD simulation in this work was performed at an extremely low temperature, very different from the 'ordinary' conditions of experiments or measurements, so the dynamic features of the circular graphene nanoflake oscillator are presented in an ideal situation. This simulation work explicitly demonstrated that graphene nanoflake oscillators are applicable to nanoscale sensors, actuators, resonators, motors, engines, filters, memories and switching devices, and quantum computing, as well as

ultra-fast-response oscillators. A very high level of vacancy is required in such a graphene nanoflake device to protect the graphene nanoflake sample from the measured environment. Further work should include quantum mechanics analyses to reveal structural and electronic properties of unusual carbon nanostructures, electron transport properties, and the influence of electric and magnetic fields. Although the interpretation of modern quantum theory seems still to be an open question, in most cases quantum theory is necessary for the description of the organization of forms of matter. Thus, quantum mechanics should be included in future work to address the structural and electronic properties of unusual carbon nanostructures, electron transport properties, and the influence of electric and magnetic fields.

4 CONCLUDING REMARKS

We investigated the oscillator behaviors of a square graphene nanoflake with triple layers in retracting motions by performing classical MD simulations. The oscillatory behaviors of the square graphene nanoflake were damped rapidly with increasing MD time. While the translational motions of the square graphene nanoflake were damped quickly, the rotational motions remained for a long time and its full rotation was found sometimes. The initial kinetic energy of the axial translational motion was changed into the energy of orthogonal vibrational and rotational motions. As the initial velocity of the square graphene nanoflake oscillator increased, its telescoping region increased, then its structural asymmetry along the translational axis due to its own small rotation exerted asymmetric vdW force on it, and finally, this asymmetric vdW force increased its rotational motions during the axial translational motions. This rapid damping of its translational motions revealed that graphene-flake oscillators have a weakness to become stable translational motion oscillators because of very low quality factors in the translational motions. However, such graphene flakes have great potential as core components in NEMSs by detecting their motions with ultrahigh sensitivity to facilitate the development of sensors, memory, and quantum computing.

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