A Graphene-based Nanoparticle Motion Converter

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Abstract

Van der Waals force generated by different nanoparticles (fullerenes and carbon nanotubes) on graphene substrates through shape curvature gradient is discussed in this paper, which drives the directional movement of nanoparticles, and provides a method for realizing the reciprocating movement of nanoparticles. The nanoparticles can move periodically on graphene substrates by means of two-end driving. In the future, it may be possible to provide a way for the construction of nano-scale high-frequency switches and nano-machines.

Keywords

Graphene; Nanoscale converter; Molecular dynamics.

1. Introduction

The macro world is full of various types of motion, among which there are motion conversion, such as gear transmission, chain transmission, shaft transmission and so on. Similarly, in the micro-world, such as nano-scale, there are corresponding motions. Directional motions driven by various energy sources (including temperature gradient, pressure, stiffness, surface chemistry, etc.) have been extensively studied[1-3]. Surface bending can lead to changes in physical interactions[4-8], especially the van der Waals force between water molecules and curved graphene layers[9], which decreases with the decrease of curvature. Based on this mechanism, a nanometer device consisting of nanoparticles and graphene substrates is constructed. The curvature of graphene substrates is changed by the movement of graphene substrates atoms, which in turn affects the van der Waals force between nanoparticles and substrates. Once the curvature gradient of the substrate is formed, the van der Waals force gradient will follow, and then the net van der Waals force on the nanoparticles will be generated, which drives the nanoparticles to move on the graphene substrate. In this way, the atomic motion of graphene substrate is transformed into the motion of nanoparticles. At the same time, we assume that different nanoparticles may move differently under the same curvature gradient. Therefore, we use two kinds of nanoparticles: fullerene nanoparticles and carbon nanotubes nanoparticles. For fullerene nanoparticles, we choose some different sizes, such as C60, C72, C180, C240, C260. For carbon nanotube particles, we investigated the combination of single and two carbon nanotubes. Next, we use the van der Waals force generated by the shape curvature gradient to orientate the movement of nanoparticles. And try to make the nanoparticles can move back and forth.

2. Models and methods

Based on molecular dynamics, Lammps is used for simulation. The constructed motion converter consists of a graphene substrate and nanoparticles placed on it. Among them, the graphene substrate is 30 nm long and 10 nm wide, and its armrest edge is along the x-axis. The nanoparticles are replaced by single fullerenes (C60, C72, C180, C240, C260) and then carbon nanotubes (chiral n5m5, 3nm long, transversely placed). Initial relative position: If the nanoparticles are fullerenes, refer to Fig. 1, x direction, the distance between the fullerenes center and the left end of graphene substrate is 2 nm, the Y direction is centered on the graphene substrate, and the distance between the Z direction fullerenes center and graphene substrate is the radius of the fullerenes plus 0.34 nm; if the nanoparticles are single carbon nanotubes, refer to Fig. 2, chirality is n5m5, length is 3 nm, transversely placed. The left end of the carbon nanotubes in the X direction is 2 nm from the left end of the graphene substrate, and the center of the Y direction is placed on the graphene substrate. The axis of the carbon nanotubes in the Z direction is 0.34 nm from the graphene substrate. If the nanoparticles are replaced by double carbon nanotubes, referring to Fig. 3, the chirality of the two carbon nanotubes is n5m5, 3 nm in length, and the left end of the carbon nanotubes is 0.34 nm from the graphene base. The left end of the plate is 2 nm, the axis of carbon nanotubes in Y direction is 2 nm away from the center of graphene substrate, and the axis of carbon nanotubes in Z direction is 0.34 nm away from graphene substrate. Constraints: Since the constraints of more than three models are the same, the constraints are shown in Figure 3. The four apex angles (yellow region) of the graphene substrate are all connected with the linear springs in the X and Z directions of the atoms in the 1X1nm2 region, and the elastic coefficients are 10N/m. REBO force field is used in the molecule and Van der Waals force field is used in the molecule. The parameters are e=2.968 meV and_=0.3407 nm. First, the nanoparticles were heated for 0.2 ns at 300 K of NVT ensemble temperature, while ensuring that the nanoparticles did not move along the X direction. After that, the centroid restriction of nanoparticles was removed, and NVE ensemble was used to simulate the movement of nanoparticles on graphene substrates. Driving operation: There are two operation areas, left operation area (blue area, center position, size 1X1nm2) and right operation area (black area, center position, size 1X1nm2). Here we use alternating cycle control at both ends to drive operation. We define a cycle operation as follows: the right operation area is away from the initial position in the negative direction of z, moving uniformly for 2ns, co-location. After that, it moves 4 nm to the initial position in the positive direction of Z. It moves 2 ns at a uniform speed and 4 nm at a total displacement. Then the left operating region moves 2 ns at a uniform speed in the negative direction of Z and 4 nm at a total displacement. Then it moves 2 ns at a uniform speed in the positive direction of Z and 4 nm at a total displacement. Then repeat the above multiple cycle operations.

Fig. 1 Fullerene nanoparticles

Fig. 2 Single carbon nanotubes

Fig. 3 Replacement of nanoparticles with double carbon nanotubes

3. Results

Periodically driving the operating region, i.e. the periodic motion of graphene substrate in Z direction, will drive the nanoparticles to and fro in X direction. More specifically, when the operating area is far from the initial position, this end will bend, because the other end is completely flat, then a curvature gradient will be generated in the X direction of the flat end and the bending end. Such a curvature gradient makes the van der Waals force between nanoparticles and graphene substrates have a gradient, which makes the nanoparticles move in the direction of increasing curvature. Finally, the nanoparticles slip to the bending end for attenuation oscillation. As the operating region approaches the initial position, most of the nanoparticles will be adsorbed by the edge of the bending end, and the x-direction displacement is not obvious. Some of the nanoparticles escape from the adsorption of the edge and slide to the other end.

From the following illustration, you can see that

(1) Periodic synchronous movement, the synchronization effect between the operation area and the nanoparticle movement can be achieved.

(2) Vertical motion conversion, the motion of graphene substrate in Z direction is converted to that of nanoparticles in X direction, and the two directions are vertical.

(3) Displacement amplification, the displacement of graphene substrate is 4 nm, and the nanoparticles move about 28 nm in the X direction.

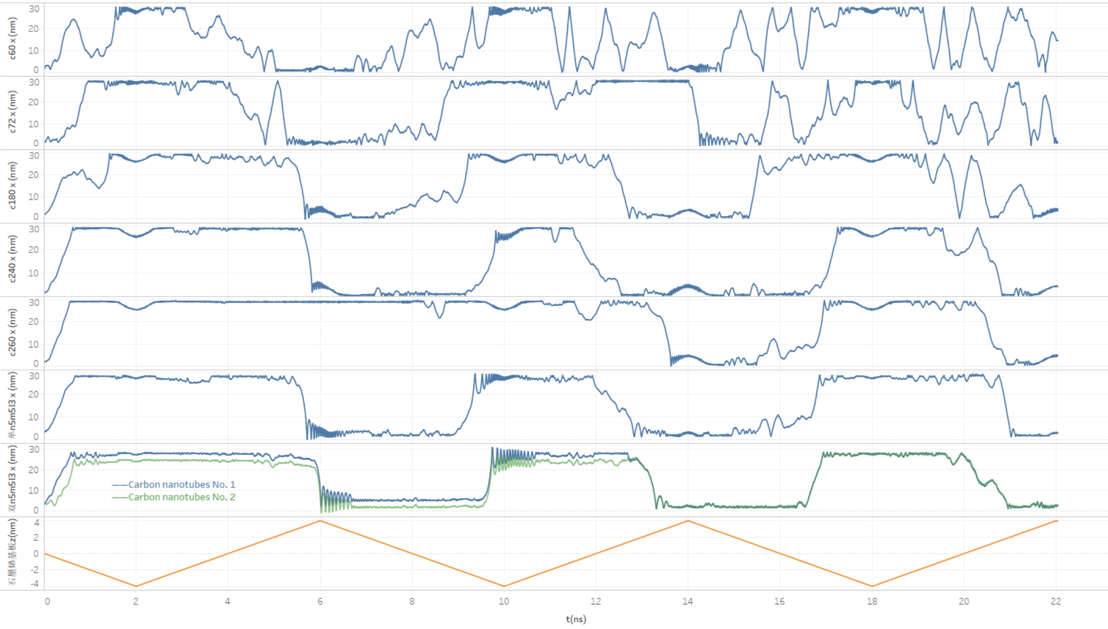

Fig. 4 X-t displacement of nanoparticles and Z-T combination diagram of graphene substrates

The yellow polyline diagram in Figure 4 shows the displacement of graphene substrate in Z direction. It also stipulates that when the polyline corresponds to the negative Z coordinate, it represents the movement of the right operating area, and when the polyline corresponds to the positive Z coordinate, it represents the movement of the left operating area. Here we find that the periodic motion of fullerene c240, single carbon nanotubes and double carbon nanotubes are clearly distinguished. The analysis of their motion properties (displacement, velocity and acceleration in X direction) shows that the velocity and acceleration of fullerene c240, single carbon nanotubes and double carbon nanotubes fluctuate more steadily in most of the time, but they fluctuate more when they are near the bending end. This is because nanoparticles are far from the equilibrium position of the substrate. The particles will slide towards the bending end of the substrate, and when the substrate reaches the farthest point away from the initial position, the velocity of the nanoparticles will reach the maximum, and at this moment, it will oscillate violently back and forth. Therefore, velocity and acceleration fluctuate more at this location than at other locations. For Figure 7, there is a fixed displacement difference between CNTs and CNTs before 13ns, and the displacement difference disappears after 13ns. The x-t curve of CNTs coincides with that of CNTs after 13ns. This is because, in the period before 13ns, the two carbon nanotubes are joined at the end of the head and the end, and after 13ns, the two move side by side. Only when they are attracted to each other can the shape trend of the x-t curve be consistent.

Fig. 8 shows the corresponding motion position of fullerene C240 at the first 8 ns interval of 1 ns. In short, in these three cases, the velocity and acceleration are relatively stable except for fluctuating distances at certain locations.

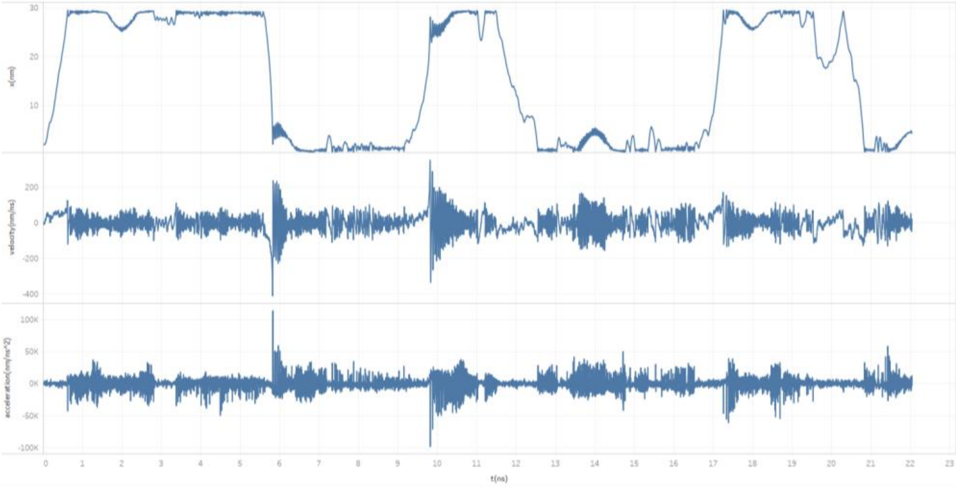

Fig. 5 Kinematic properties of fullerene C 240

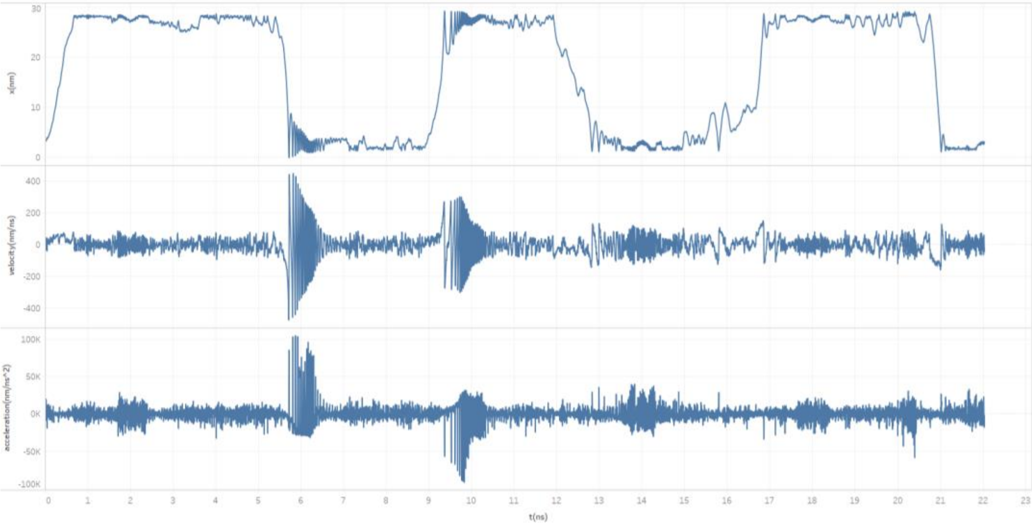

Fig. 6 Kinematic properties of single carbon nanotubes (n5m5)

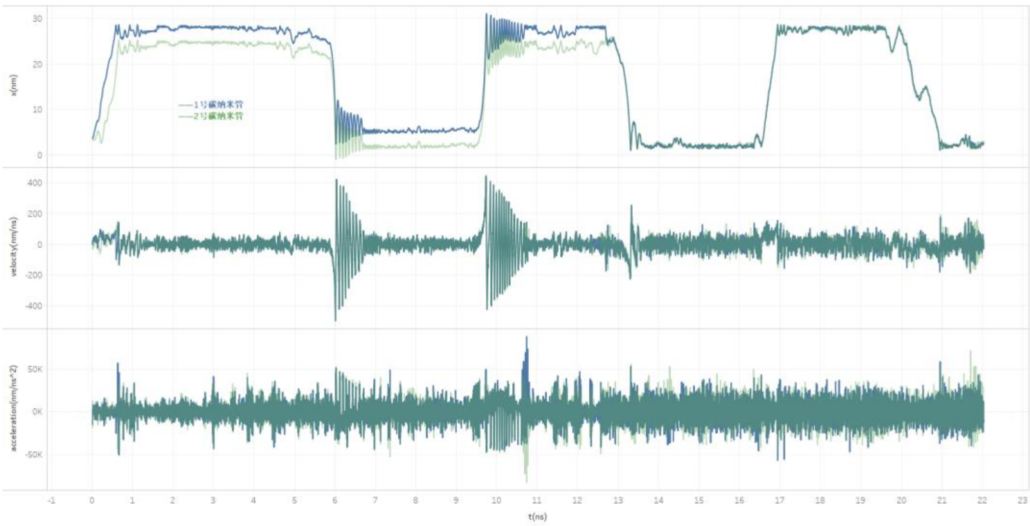

Fig. 7 Kinematic properties of double carbon nanotubes (n5m5)

4. Conclusion

By comparing the two kinds of nanoparticles, we found that most of them can move back and forth on graphene substrates through double tails. This structure may provide the possibility for the construction of high-frequency nanoswitches, nanoparticle transport or nanorobot components.

Acknowledgments

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