Molecular Dynamics Simulation of Nanoparticle Transport

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Abstract

In a non-uniform electric field, different unidirectional water flows of different sizes are generated in different pipe diameters[1-3], so it is desirable to use this water flow to push the particles to orientate. The fullerene was selected for the moving particles, and the (10,10), (12,12), (15,15), (18,18) type single-walled carbon nanotubes were selected as the transport channels of fullerenes in the nanometer amount[4]. The class of medium-nano electromechanical systems has been applied to a number of applications, such as nanomotors. The non-uniform electric field is mainly driven by an electric field with a slope of 0.1 to drive the fullerene. In this chapter, the directional motion of fullerenes based on carbon nanotubes as transport channels is mainly described in detail. The carbon nanotubes are filled with water molecules[5-7], and there are two water droplets on each side of the graphene, and the number of water droplets on both sides is the same. The motion of fullerenes in carbon nanotubes with different diameters was studied and analyzed.

Keywords

Molecular Dynamics Simulation, Nanoparticle Transport.

1. Introduction

Inspired by previous molecular motor research, here we provide four models. 10 nm (10,10) carbon nanotubes, 10 nm (12,12) carbon nanotubes, 10 nm (15,15) carbon nanotubes, and 10 nm (18,18) carbon nanometers tube. Among the (10,10), (12,12), (15,15), (18,18) type carbon nanotubes, fullerene beads are placed, and fullerene beads are placed on the left end of the carbon nanotubes. The distance to the tube wall is about 0.15 nm, and a drop of water is placed at a distance of 0.3 nm from the graphene plate, for a total of 3921 water molecules. A non-uniform electric field is added to the overall structure, the direction of the electric field is z-direction, and the direction of the x-axis is continuously increased[8-10]. The motion of the fullerene spheres in the carbon nanotubes is observed by adding a non-uniform electric field. A graphene plate is placed on each end of the carbon nanotube to achieve the effect that water can only pass through the carbon nanotube[11]. Both carbon nanotubes and both ends of the graphene plate are filled with water. The water molecules are driven by a non-uniform electric field, thereby driving the directional movement of the fullerene beads in the carbon nanotubes[12].

Figure 1-1 shows the combined structure of (10,10) type carbon nanotubes and fullerenes, graphene sheets and water droplets; Figure1-2 shows (12,12) type carbon nanotubes and fullerenes, graphene sheets. And a combined structure of water droplets; Figure1-3 is a combined structure of (12,12) type carbon nanotubes and fullerenes, graphene sheets and water droplets; Figure 3-4 is (15,15) type carbon nanotubes and rich The combined structure of olefins, graphene sheets and water droplets; Figure 1-4 is the combined structure of (18,18) type carbon nanotubes and fullerenes, graphene sheets and water droplets; it can be clearly seen from the figure (6 , 6) and (8,8) type carbon nanotubes are not filled with fullerenes, because the diameter of fullerenes is larger than the diameter of (6,6) type carbon nanotubes, can not be forced into the tube Among them, its role is mainly used to study the change of water flow in the tube after adding a non-uniform electric field.

Fig1- 1 type carbon nanotubes

Fig1- 2 (12,12) type carbon nanotubes

Fig1- 3 (15,15) type carbon nanotubes

Fig1- 4 (18,18) type carbon nanotubes

The structure is still simulated by molecular dynamics. The software of GROMACS 4.0.7 is used to do the molecular dynamics simulation, and the running results are step by step, and the generation of the top file is emphasized. The top file is carbon. The top of the nanotube, the top of the fullerene and the top of the graphene are combined to form a top file that is not generated by the whole result. If the entire structure generates a top file, a large number of errors will occur, and the generated one is wrong. The two ensembles used here are the micro-regular ensemble and the regular ensemble (NVT). When using the micro-regular ensemble, the number of atoms (N), volume (V) and energy (E) are always constant. . When using the regular ensemble, the atomic number (N), volume (V) and temperature are always constant. The temperature is always maintained at 300 K. Tip3p is a model used for water molecules. Because the structure is placed under a non-uniform electric field, it is necessary to know whether the water molecule model of tip3p is reasonable. The water molecule model of tip3p is reasonable when the electric field strength is less than 10V/nm.

2. Results and Discussion

The structural diagrams of the (10,10), (12,12), (15,15), and (18,18) systems from the initial structure to equilibrium after 20 nanosecond calculations are given. It can be clearly seen that at the beginning of the fullerene sphere at the leftmost end of the carbon nanotube, after 20 ns of calculation, the fullerene sphere is orientated to the right end of the carbon nanotube.

In the initial stage of the structure, the fullerene spheres are oriented at the leftmost end of the carbon nanotubes, and the fullerene spheres are orientated to the rightmost end after 20 ns of calculation. Because the diameter of the (10,10) type carbon nanotubes is not much larger than the diameter of the fullerene spheres, so that the water molecules driven by the non-uniform electric field cannot be between the carbon nanotubes and the fullerene spheres. Passed in the gap, so the most

computationally short time can achieve the desired effect. Compared with the (12,12), (15,15), (18,18) type carbon nanotubes, because the diameter is much larger than the fullerene spheres, the water molecules driven by the non-uniform electric field can be from the gap. Passed, so the expected effect was not achieved in a short period of time.

Figure 1-5 shows the structure of the (10,10) type carbon nanotubes and fullerenes without molecular dynamics simulation. It is obvious that fullerenes are at the left end of the carbon nanotubes. Figure 1-6 is a structural diagram after 20 ns of molecular dynamics. It is obvious that the fullerene sphere has moved to the right end of the carbon nanotube. Carbon nanotubes of type (10,10) are the most effective of all structures. Figure 1-7 shows the structure of the (12,12) type carbon nanotubes and fullerenes without molecular dynamics simulation. The fullerenes are still placed at the leftmost end of the carbon nanotubes. Figure 1-8 shows a structural diagram of the combination after 20 ns, and the fullerenes move significantly to the right. Figure 1-9 shows the structure of the (15,15) type carbon nanotubes and fullerenes without molecular dynamics simulation. The fullerenes are still placed at the leftmost end of the carbon nanotubes. Figure 1-10 shows a structural diagram of the combination after 20 ns, and the fullerenes move significantly to the right.

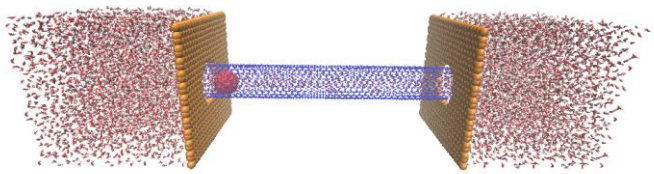

Fig1- 5(10,10) type before simulation

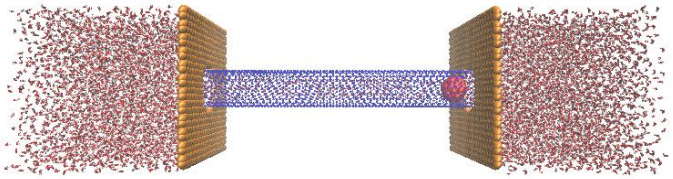

Fig1-6 The initial structure of (10,10) and the structure after simulating 20ns

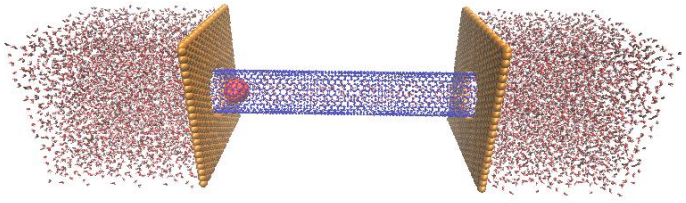

Fig 1- 7 (12,12) type before simulation

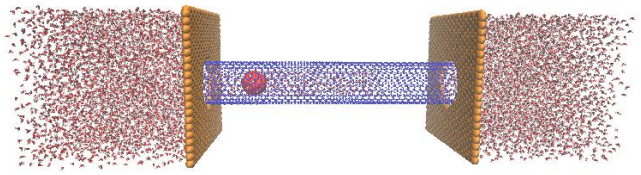

Fig1- 8 The initial structure of (12,12) and the structure after simulating 20ns

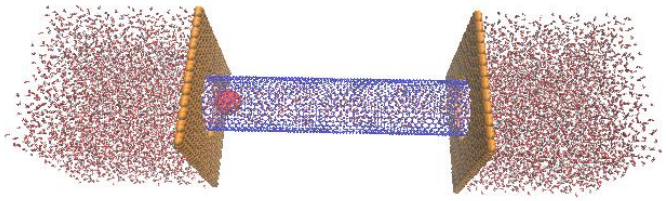

Fig1- 9 (15,15) type before simulation

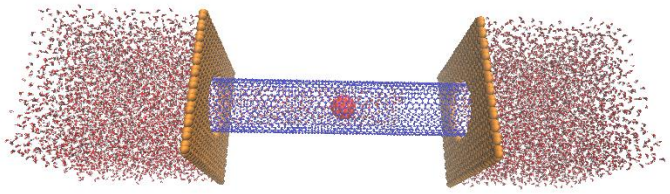

Fig 1- 10 The initial structure of (10,10) and the structure after simulating 20ns

The fullerene sphere is electrically neutral, and the reason why it can be orientated is that the water molecule is driven to move in an orientated direction, so that the water molecules drive the fullerene sphere to achieve the directional motion. The movement of fullerene spheres in (10,10), (12,12), (15,15), (18,18) type carbon nanotubes, in (10,10) type carbon nanotubes The speed is much faster than that of the (12, 12), (15, 15), and (18, 18) carbon nanotubes. Transportation efficiency is clearly more obvious.

After the molecular dynamics simulation, the output data is analyzed. The system has a significant change in the water flow in the X direction after the upper non-uniform electric field.

From the above analysis, the fullerene spheres are bound in the carbon nanotubes, so the movement of the fullerenes in the carbon nanotubes is not affected by the thermal perturbation of the water molecules. It will be found that the water molecules in the carbon nanotubes are slightly reduced, but the structure of the water is not destroyed, which is more obvious in the (6,6) type and (10,10) type carbon nanotubes because it averages every nanosecond. There will be about 17 water molecules passing through. This can effectively drive the movement of fullerenes.

Figure 1-11 shows the motion law of the centroid, because the non-uniform electric field is applied along the z direction, and the fullerene moves in the positive z-axis direction and oscillates in the x and y directions. Mainly to view the law of motion in the z direction. In the motion diagram of fullerene in (10,10) type carbon nanotubes, it can be clearly seen that at the 10th ns, the fullerenes

have moved 10nm to reach the rightmost end of the carbon nanotubes, and the slope of the change is relatively large. It shows that the fullerene moves rapidly in the (10,10) type carbon nanotubes at a rate of 1 nm⁄ns, that is, its average nanosecond shift is 1 nm in the positive direction of the z-axis. In the motion diagram of fullerene in (12,12) type carbon nanotubes, x and y have a relatively large moving range, and the average sway is about 0.4 nm. The general trend of fullerenes in the z direction is to move to the right. However, in these 20 ns, fullerenes did not reach the rightmost end of the carbon nanotubes. Moreover, its moving speed to the right is very slow, and its velocity averages 0.2 nm⁄ns, that is, its average no nanosecond moves 0.2 nm in the positive direction of the z-axis. In the motion diagram of fullerene in (15,15) type carbon nanotubes, although the amplitude of the centroid x, y is not very large, the amplitude of the left and right sway is about 0.1 nm, but it is a moving trend in the z direction. It is moving in the positive direction of the z-axis, but it is more severe in the z-direction. In these 20ns, fullerenes also did not reach the rightmost end of the carbon nanotubes. The fullerene shifted to the right with a slow tendency. The average velocity and the velocity of the (12,12) type fullerene were almost 0.2nm⁄ns. . In the motion diagram of fullerene in (15,15) type carbon nanotubes, the sloshing of 13ns in the first 7ns fullerene is much smaller, about 0.5nm, and its mass center x in the last 13ns. The y shake amplitude is about 1 nm.

The largest unidirectional flux of water is the (6,6) type carbon nanotubes, which are single-chain water molecules moving inside, followed by one-way circulation in (10,10) type carbon nanotubes. Since fullerenes cannot be placed in (6,6) type carbon nanotubes, fullerene is placed in (10,10), (12,12), (15,15), (18,18) type carbons. In nanotubes, water molecules cannot pass through the gap between fullerenes and carbon nanotubes in (10,10) type carbon nanotubes, at (12, 12), (15, 15), (18, 18) Water molecules in the carbon nanotubes can pass through the gap between the fullerene and the carbon nanotubes.

In the data analysis diagrams after simulating these four structures, it can be concluded that among these four structures, fullerene has the fastest movement speed in the (10,10) type carbon nanotubes, and it is in x, In the y direction, the amplitude of movement in the x and y directions is smaller than that of the other three structures. This is because the distance from the tube wall of the carbon nanotube to the fullerene is very close, which has a great binding effect, so it will appear This effect. (12, 12), (15, 15), (18, 18) These three types of carbon nanotubes, after adding a non-uniform electric field, although not reaching the rightmost end at 20 ns, the overall trend is to the z-axis Moving in the positive direction, so this place is a bit negligent, and it is necessary to perform molecular dynamics simulations on these three structures for at least 40 ns. Fullerene will also reach the right end of the carbon nanotubes under long-term simulation.

The movement rate of fullerenes is proportional to the size of the one-way water flow in the carbon nanotubes. When the one-way water flow is hit, the fullerene moves at a faster speed, and the time to reach the desired position is short, so the loss The efficiency will be very high. There is also a very important relationship between the diameter of the particles and the diameter of the carbon nanotubes. If the type and size of the particles are determined, the selection of the transport channels (carbon nanotubes) must be selected. The diameter of the pipe is larger than that of the granules, or it is impossible to transport the granules, but it is necessary to determine the maximum transport efficiency when it is large. Through these several simulations, the carbon nanotubes and the transported granules can be obtained. The distance between them is extremely important for its transport efficiency. When the distance between the two is large, water molecules will pass through this gap in a large amount, thereby reducing the force on the particles, so the transport of the particles. The speed will be very low, because the unidirectional flux at this time is very small. Through the simulation of several structures, it is found that the unidirectional flux in the crude carbon nanotubes will appear in one-way circulation for several consecutive nanoseconds. The amount is zero. Then the particles will not have good transport efficiency.

Although the simulation is only for the four structures, the basic effects are similar to the expected effects. Although the subsequent need to simulate a longer variety of structures for a longer period of

time, the effect is better. Including the carbon nanotubes that can be made in (9, 9), (11, 11), (13, 13) type, the same simulation is performed to more precisely explain the movement of the particles in their tubes.

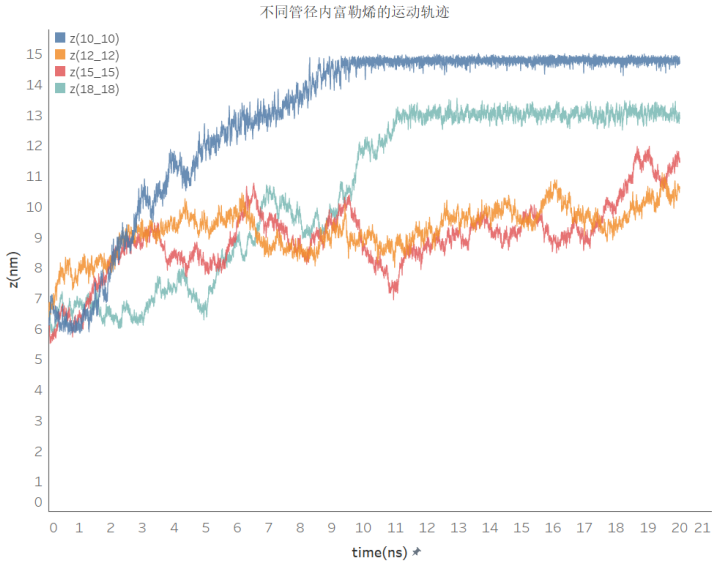

Fig1- 5 Motion Analysis of Fullerene in (10,10) Type Carbon Nanotubes

3. Conclusion

The fullerene pellets are placed in carbon nanotubes of different diameters (10, 10), (12, 12), (15, 15), (18, 18). At the 10th ns of the (10,10) type carbon nanotubes, the fullerene has moved 10 nm to reach the rightmost end of the carbon nanotube, and the slope of the change is relatively large. In the (12,12) type carbon nanotube fullerene, the range of x and y is relatively large, and the average back and forth sway is about 0.4 nm. The general trend of fullerene in the z direction in the z direction is to move to the right. In the (15,15) type carbon nanotubes, the fullerene center of mass x, y sloshing amplitude is not very large, and the amplitude of the left and right sway is about 0.1 nm, but in the z direction, although the moving tendency is moving in the positive direction of the z axis However, it is more serious to sway back and forth in the z direction.

Acknowledgments

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