NANO LETTERS

2006
Vol. 6, No. 9
1893−1895

Nanopumping Using Carbon Nanotubes

Zeke Insepov,* Dieter Wolf,† and Ahmed Hassanein

Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439

Received April 25, 2006; Revised Manuscript Received June 13, 2006

ABSTRACT

A new "nanopumping" effect consisting of the activation of an axial gas flow inside a carbon nanotube by producing Rayleigh traveling waves on the nanotube surface is predicted. The driving force for the new effect is the friction between the gas particles and the nanotube walls. A molecular dynamics simulation of the new effect was carried out showing macroscopic flows of atomic and molecular hydrogen and helium gases in a carbon nanotube.

Actuation of a fluid flow in microcapillaries has fundamental interest in the areas of nanorobotics, fine-printing at the nanoscale level, atom optics, quantum computing, hydrogen energetics, chemical process control, cell biology, medical drug delivery, and molecular medicine.[1] Microflow control is also important for commercial applications: DNA analysis, drug screening, optical display technologies, and tunable fiber optic waveguides, thermal management of semiconductor devices and lasers, clinical and forensic analysis, and environmental monitoring.[2] Study of fluid flows in narrow channels has become a hot area of research since the discovery of nanotubes by Ijima in 1991. The microflow systems include liquid flows in narrow slit-pores,[3] very thin liquid films on solid surfaces,[4] flows in micropumps, microarrays, and membranes.[5,6] Fluid-flow dynamics in carbon nanotubes has been studied in ref 7. Interaction of fluids with microscopic pores by filling (imbibition) of nanotubes with gases or liquids is of great technological interest;[9] various methods for atomic pumping through carbon nanotubes were proposed in refs 11 and 12. In ref 11, a laser-driven pump for atomic transport through a carbon nanotube (CNT) was proposed based on the generation of electric current through the tube, which in turn would move ions in it by drag forces. A nanopipet concept for dragging metal ions through a multiwalled CNT was confirmed experimentally.[12] Hydrogen storage and a feasible isotope separation method by a carbon nanotube is discussed in refs 13 and 14. Liberation of the atomic form of hydrogen chemisorbed on carbon materials is discussed in refs 15 and 16. This process is very important for future hydrogen application in the car industry. Even if the Department of Energy target of 6.5 wt % of hydrogen storage is reachable, for example, by a chemisorption mechanism, then the subsequent liberation of hydrogen by heating will need very high temperatures, which makes this application unrealistic.

Contrary to the dense fluid flows in micrometer- and nanometer-sized channels, rarefied gas flows are of interest for future gas pumping. Microelectromechanical systems and microscale vacuum technology devices are yet another area of applications.[17−20] Molecular dynamics (MD) and Monte Carlo (MC) methods were applied for studying microfluids.[3,4,7−10,13,14] Atomistic simulations of microfluid flows in nanochannels are rather limited.

Propagation of surface acoustic waves on metal cylinders with finite lengths and through the carbon nanotubes were discussed in refs 21−24. There are a few ways to activate surface-traveling waves on the nanotube surface. One way is to use short laser pulses to generate thermoacoustic waves on a tube.[25] Another way is to send ultrasound waves through the liquid or dense gaseous media to the nanotube.[26] Rayleigh surface waves are activated when a longitudinal wave traveling in a liquid/gas impinges on a solid surface at an incidence angle equal to the Rayleigh angle θ (where $\theta = \arcsin(C_p/C_s)$, C_p is the velocity of the incident wave and C_s is the velocity of the surface wave in the material.[26]

Propagation of the specific traveling waves on the dolphin skin surface is discussed in refs 27 and 28.

The goal of this paper is to prove the nanopumping concept by MD simulation of a carbon nanotube device that will enable pumping gases and/or liquids at the nanoscale level, through the nanometer channels. A simple MD simulation model of the gas−nanotube interaction was developed when the nanotube walls were moving in accordance with the Rayleigh surface-traveling wave. This model is used to simulate the macroscopic flow of a few gases lighter than carbon (hydrogen, helium) inside the carbon nanotubes activated with the surface waves. The atomic flow rate and average velocity of the gas flow through the nanotube was calculated to verify the overall concept and the efficiency of the nanopumping.

As an input structure for the MD simulations, coordinates of the zigzag nanotube carbon atoms were generated. Tersoff[29] and Brenner[30] interaction potentials were employed

* Corresponding author. Phone: 630-252-5049. E-mail: insepov@anl.gov.
† Present address: Idaho National Laboratory, P.O. Box 1625, MS 2211 Idaho Falls, ID 83415-2211.

10.1021/nl060932m CCC: $33.50
Published on Web 07/27/2006

Table 1. Parameters of Lennard-Jones Interaction Potentials for Various Gases and Carbon

gases	LJ radius, σ (Å)	LJ depth, ϵ (K)	reference
H_2-H_2 interaction via Solvera−Goldman potential	3.41	34.3	14
H_2-H_2	2.97	33.3	31
H_2-C	3.19	30.5	
H_2-H_2	2.958	36.7	32
H_2-C	3.179	32.05	
H_2-H_2	2.958	36.7	33
H_2-C	3.179	32.17	
He−He	2.74	16.24	13
He−He	2.633	10.87	7
He−C	3.191	19.3	

to describe the carbon−carbon interactions. Various gases interacting via Lennard-Jones potentials with the parameters given in Table 1 were placed inside the nanotube. The system was brought into equilibrium at room temperature and the Rayleigh transverse surface waves, with a phase velocity of about 22 km/s, were generated by sending the traveling waves with $f = 10^6-10^{13}$ Hz along the nanotube. The carbon displacements were perpendicular to the axial direction of wave propagation (so the nanotube vibrations occurred in radial directions). The radial amplitudes of the waves were chosen to be in the interval of 1−5% of the nanotube radii.

We have placed 128 or 256 gas atoms with four different masses (lighter than carbon) inside the nanotube and by applying a traveling wave along the nanotube surface. Our MD simulation explicitly incorporates the interaction between the gas atoms and the nanotube and its effect on the gas flow. The interactions between the gas atoms and the nanotube carbon atoms and the gas atomic masses have been chosen such that the gas did not penetrate through the nanotube walls, even at high velocities. The following chirality numbers of the nanotubes have been tested: (5 × 0), (15 × 0), (10 × 0), and (15 × 15). The total length of the nanotubes was equal to 100 Å, and their diameters were 10−20 Å. Depending on the total number of gas atoms inside the nanotube, the real simulation time was about 35 ps.

According to our simulation results shown in Figure 1, the gas atoms inside the nanotube move almost freely, along the ballistic trajectories, and they are easily accelerated to a very high axial velocity, along the direction of the traveling wave as a result of multiple synchronous collisions with the moving (traveling) nanotube walls.

Figure 1 demonstrates the nanopumping effect for 256 He atoms (shown by red color) that were placed inside a L = 100 Å long carbon nanotube (carbon atoms are shown in gray color), with a diameter of 12 Å.

The nanotube has a chirality of (15 × 0) and was built of 1410 carbon atoms. After activating the surface-traveling wave, with a frequency of 10 THz and a phase velocity of 22 km/s, the helium atoms started to move in the direction of the wave propagation (in Figure 1, from left to right). Various instants are shown from an initial 44 fs (Figure 1a) to final at 18 ps (Figure 1e). (See also the Supporting Information: movies S1 and S2 for this simulation and movies S3 and S4 for the simulation of 128 He atoms in a nanotube.)

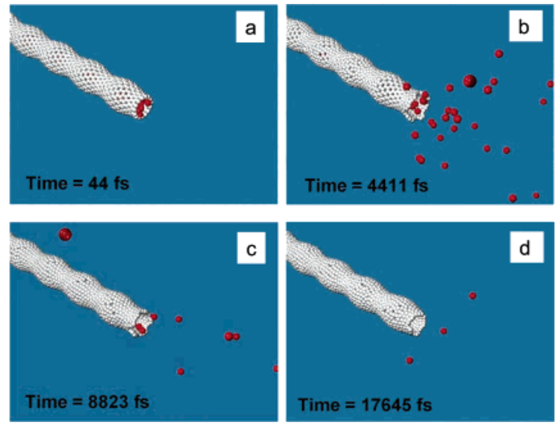

Figure 1. Various instants (from left to right) are shown from an initial 44 fs (a) to final at 17.6 ps (d).

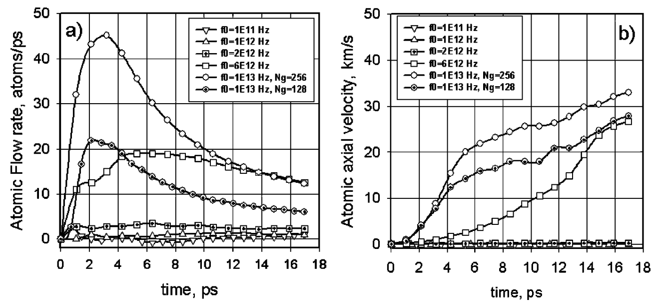

Figure 2. (a) Dependence of flow rate through the activated nanotubes on the simulation time for various wave frequencies: $10^{11}-10^{13}$ Hz. (b) The average flow velocity vs time for various wave frequencies (1 atom/ps = 2.4 × 10^{-4} sccm).

Atomic fluxes generated due to the nanopumping effect for various frequencies of the surface waves for the gas initially at rest ($<v> = 0$) are shown in Figure 2a. The total flux increases up to a few picoseconds and then decreases because of the depletion of the gas inside the tube. The average axial velocities of helium atoms are given in Figure 2b for different wave frequencies. The velocity is rather small below ~1 THz. At 6 THz the velocity reaches a hyperthermal value of ~30 km/s, as the kinetic energy of the atoms becomes larger than thermal energy k_BT.

The frequency dependence of the flow rate though the nanopump is given in Figure 3a, and it will depend on the total nanotube length. Because the nanotube length was chosen to be 100 Å, the characteristic frequency is rather high. The maximum effect is seen at approximately 38 THz. Figure 3b shows the dependence of the nanopumping effect on the ratio L/λ where λ the wavelength of the surface wave.

There is at least one physical effect that closely resembles the nanopumping effect. The well-known Fermi acceleration of cosmic rays occurs when an energetic ion passes through areas with periodic magnetic fields. The Fermi acceleration is zero if the initial ion velocity is zero. Contrary to the Fermi acceleration, the nanopumping occurs in a gas at rest, with zero average velocity, for which the Fermi effect is zero.

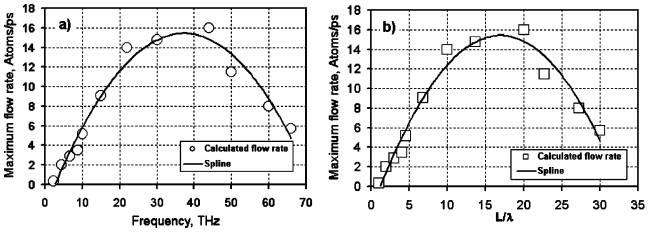

Figure 3. Nanopumping effect strongly depends on the wave frequency. (a) The dependence of the maximum flow rate on the frequency of the traveling wave; (b) the dependence of the flow rate on the ratio L/λ.

We believe that our simulation of nanopumping through carbon nanotubes containing gas atoms and having the walls vibrated in accordance with the Rayleigh traveling wave law confirms our concept. If this hypothesis is true, then the pumping effect could be used for fueling laptop computers, which is a serious engineering problem. Another example is gas pumping. Application of the new idea to the development of new turbo molecular pumps would certainly increase the pumping efficiency.

The predicted effect has similarity in live nature, for example with the skin features of fast-swimming sea animals, such as dolphins. There are some indications that dolphins use specific (traveling) waves on their skin surface to damp the turbulence in the boundary layers near the skin surface. However, such mechanisms involving compliant surfaces are not yet well understood.[27,28]

We showed that after the Rayleigh surface wave is activated the gas inside the carbon nanotube experiences multiple reflections from the nanotube walls. At a certain combination of the atomic masses, wave frequency, and phase velocity, the gas inside the nanotube starts flowing with a macroscopic high velocity, in the direction of the traveling surface wave, which we have called "nanopumping". The driving force for the new effect is the friction between the gas particles and the nanotube walls. A molecular dynamics model of the nanopumping effect was developed for a nanotube filled with various gas particles and the gas flows of atomic and molecular hydrogen and helium gases in a CNT were calculated. Flow rates were calculated at various frequencies and phase velocities of the surface waves. The proposed nanopumping effect is a new physical phenomenon that reveals itself at the nanoscale level. We believe that similar effects should exist for larger space/time scales.

Supporting Information Available: Movies S1−S4. This material is available free of charge via the Internet at http://pubs.acs.org.

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NL060932M