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Molecular Dynamics Simulations of a Linear Nanomotor Driven by Thermophoretic Forces

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We conduct molecular dynamics simulations of a molecular linear motor consisting of coaxial carbon nanotubes with a long outer carbon nanotube confining and guiding the motion of an inner short, capsule-like nanotube. The simulations indicate that the motion of the capsule can be controlled by thermophoretic forces induced by thermal gradients. The simulations find large terminal velocities of 100–400 nm/ns for imposed thermal gradients in the range 1-3K/nm. Moreover, the results indicate that the thermophoretic force is velocity dependent and its magnitude decreases for increasing velocity.

INTRODUCTION

Thermophoresis is the motion of mass induced by thermal gradients.[1,2,3,4,5] In recent investigations thermophoresis has been used for driving solid and liquids confined inside carbon nanotubes.[6,7,8,9] Nanomotors are an attractive goal for nanotechnology.[9-13] Such nano-scale structures capable of converting thermal energy into work will be needed in many types of nanodevices, including nanoconveyors[14], memory devices[15] and nano-encapsulated material delivery systems[16,17]. Moreover to design and manufacture future molecular machines a complete understanding of the friction forces involved on the transport process at the molecular level have to be addressed.[18]

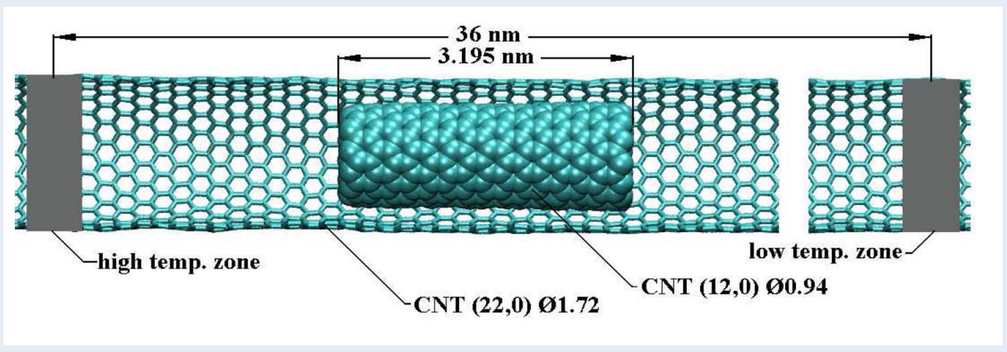

Fig. 1: Schematic of the computational setup. Cross-sectional view of the system, the outer CNT is a (22,0) zigzag CNT and the inner one is a (12,0) zigzag CNT. A thermal gradient is imposed by heating the end sections (in gray) of the outer CNT.

In recent experimental studies, Somada et al.[10] and Barreiro et al.[9] fabricated molecular linear motors consisting of co-axial carbon nanotubes (CNT). In both systems a short CNT is found to move along the axis of a long CNT, working as a molecular linear motor. Barreiro et al.[9] identified thermophoresis as the main driving mechanism for their motor, and consistent with recent numerical simulations of thermophoretic motion of gold nanoparticles and water nanodroplets confined inside carbon nanotubes[6,7]. In the experimental arrangement of Somada et al.[10] the system consisted of a capped capsule-like short carbon nanotube with a chiral vector of (12,0) encapsulated in the interior hollow space of a single wall CNT with a chiral vector of (22,0). The hollow space was approximately 8.5 nm long and limited by two fixed and inner CNTs with a chiral vector of (12,0). Somada et al.[10] proposed that the mechanism driving the capsule is related to thermal activation energy which is in equilibrium with the van der Waals (vdW) energy gain due to the interaction between the caps of the inner carbon nanotubes. They argue that the thermal energy not only activated the capsule motion but also obstructed its travel by deforming the hollow space of the system.[10] In the present work we study the ability of thermal gradients and the associated thermophoretic forces to impart motion in carbon nanotube-based linear motors.

METHODOLOGY

In this work we perform Molecular Dynamics (MD) simulations using the MD package FASTTUBE[19] to study a molecular linear motor consisting of coaxial carbon nanotubes. The system consists of an outer 42.6 nm long carbon nanotube (CNT) with a chiral vector of (22,0) corresponding to a diameter of 1.723 nm. The inner CNT is modeled as an open short 3.195 nm long carbon nanotube with a chiral vector of (12,0), and diameter 0.94 nm. We describe the valence forces within the CNT using Morse, harmonic angle and torsion potentials.[19] We include a nonbonded carbon-carbon Lennard-Jones potential to describe the vdW interaction between the carbon atoms within the double wall portion of the system. We equilibrate the system at 300K for 0.1 ns, by coupling the system to a Berendsen thermostat[20] with a time constant of 0.1 ps. After the equilibration we impose thermal gradients in the range of 0.0–4.2 K/nm by heating two zones at the ends of the outer CNT as illustrated in Fig. 1. We measure the position of the center of mass (COM) of the inner CNT during the simulation.

RESULTS

We observe, for gradients higher that 1.18K/nm, a directed motion of the capsule in the direction opposite to the imposed thermal gradient as shown in Fig. 2. For a thermal gradient of 1.18K/nm the mean terminal velocity is approximately 170 nm/ns. Moreover, we find a consistent increase in the terminal velocity for increasing thermal gradients. To confirm that the motion of the capsule is driven by thermophoresis we perform additional simulations in order to study the friction and thermophoretic forces acting on the inner CNT. In these simulations, we constrain the velocity of center of mass of the inner CNT and extract from the simulations the external forces required to drive the inner CNT for different constrained velocities and different imposed thermal gradients (Fig. 3). To measure the isothermal friction of the system we impose a zero thermal gradient while we vary the constrained COM velocity.

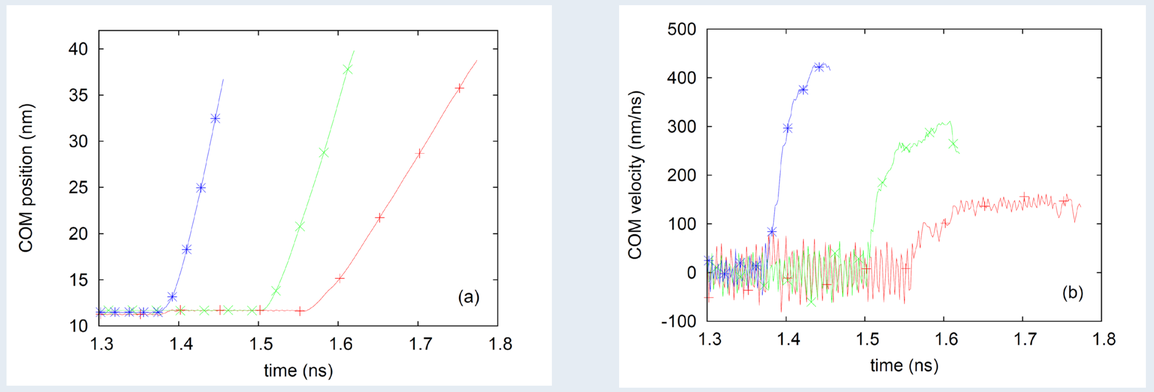

FIG. 2: Center of mass position (COM) (a) and velocity (b) as a function of time for three different thermal gradients: blue (*), 3.16K/nm; green ( ), 1.58K/nm, and red (+), 1.18K/nm.

At nonzero thermal gradients we measure the combined friction and thermophoretic forces. A positive force indicates resistance to the motion, whereas a negative force is indicative of thermophoresis. We find a systematic increase of the thermophoretic force as higher thermal gradients are imposed on the system. Furthermore, the measured isothermal friction is small compared to the thermophoretic force cf. Fig. 3b. We infer from the simulations that the magnitude of the thermophoretic force is reduced as a higher velocity is imposed to the inner CNT (Fig. 3a). We conjecture that the magnitude of the driving thermophoretic force is inversely dependent on velocity. We find that, for different imposed thermal gradients, the corresponding terminal velocity is governed by the velocity dependence of the thermophoretic force rather than a match between the thermophoretic force measured at zero velocity and the static friction. We observe from Fig. 3b that the zero external force is obtained at approximately 100 nm/ns for 1K/nm, at 250 nm/ns for 2K/nm and at 400 nm/ns for 3K/nm in reasonable agreement with the terminal velocities observed in Fig. 2b. we propose that the motion of the molecular linear motor observed in the experiments of Somada et al.[10] and Barreiro et al.[9] is primarily caused by the thermal gradient imposed on the system. We believe that our hypothesis contributes to the understanding and utilization of thermophoresis-based linear nanomotors. we hope to encourage more experimental work to study thermophoretic linear nanomotors and its potential applications.

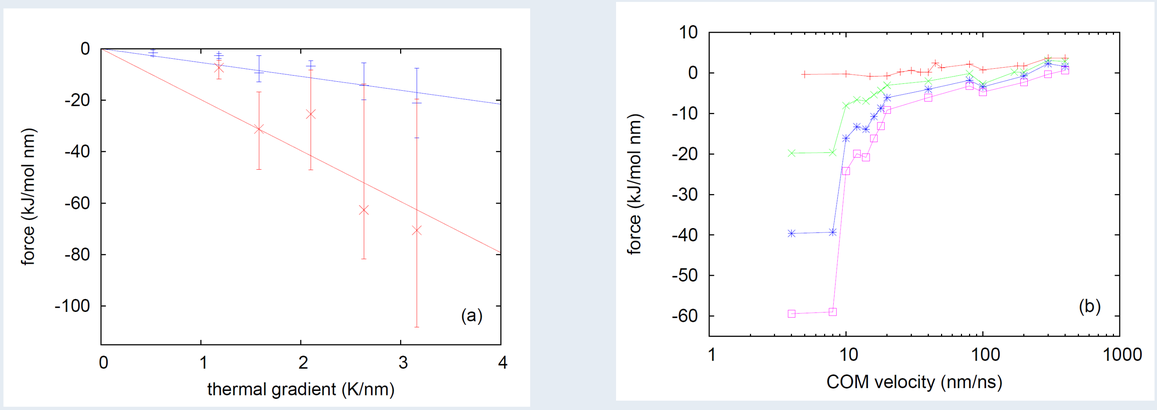

FIG. 3: External force acting on the constrained inner CNT(a) external force as a function of the imposed thermal gradient for different constrained velocities: red line and ( ), 4 nm/ns. blue line and (+), 16 nm/ns; (b) External force acting as a function of the center of mass (COM) velocity for different thermal gradients: red (+), 0.0K/nm; green ( ), 1.0K/nm; blue (*), 2.0K/nm; and fuchsia (squares), 3.0K/nm.

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