Molecular Dynamics Simulations of a Linear Nanomotor Driven by Thermophoretic Forces

Zambrano, Harvey A; Walther, Jens Honore; Jaffe, Richard L.

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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 the 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 1-3 K/nm. Moreover, the results indicate that the thermophoretic force is velocity dependent and its magnitude decreases for increasing velocity.

**RESULTS**

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.7,8 The in 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.9 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 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 FASTTUBE19 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 nondamped 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 thermostat20 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 than 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 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.