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Molecular dynamics simulations of carbon nanotube-based gears

Jie Han†, Al Globus, Richard Jaffe and Glenn Deardorff

NASA Ames Research Center, Moffett Field, CA 94035, USA

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Abstract. We use a molecular dynamics simulation to investigate the properties and design space of molecular gears fashioned from carbon nanotubes with teeth added via a benzyne reaction known to occur with C_{60}. Brenner's reactive hydrocarbon potential is used to model interatomic forces within each molecular gear. A Lennard–Jones 6–12 potential or the Buckingham (exp +6) potential plus electrostatic interaction terms are used for intermolecular interactions between gears. A number of gear and gear/shaft configurations are simulated on parallel computers. One gear is powered by forcing the atoms near the end of the nanotube to rotate, and a second gear is allowed to rotate by keeping the atoms near the end of its nanotube constrained to a cylinder. The meshing aromatic gear teeth transfer angular momentum from the powered gear to the driven gear. Results suggest that these gears can operate at up to 50–100 GHz in a vacuum at room temperature. The failure mode involves tooth slip, not bond breaking, so failed gears can be returned to operation by lowering the temperature and/or rotation rate.

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1. Introduction

The unique properties of fullerenes in dimension and topology allows one to design various nanodevices and molecular machinery parts. Figure 1 illustrates a carbon nanotube-based gear approximately two nanometers across. Shafts are single-walled carbon nanotubes and gear teeth are benzyne molecules bonded onto the nanotube. Compared with the diamonoid molecular planetary gear designed by Drexler [1], and Robertson *et al*'s fullerene based nanogear [2], the nanotube-based gears shown in figure 1 are much simpler in structure and may be synthetically accessible.

The idea of carbon nanotube-based gears comes from recent progress in fullerene science and technology. Multiwalled and single-walled nanotubes have been successfully prepared and rapid advances have been made in controlling tube diameter, length, chirality and the number of concentric shells [3]. Carbon nanotubes have many attractive material properties. For example, experiment and theory have demonstrated that nanotubes have exceptionally high Young's modulus and nanotube electronic properties vary as a function of diameter and chirality [4]. These properties have opened doors to electronic, optical, magnetic and mechanical applications. It has been shown that nanotubes can be used as atomic-scale field emitters [5], electronic switches [6], and pinning materials in high-T_c superconductors [4]. In addition, the functionality of fullerene materials provides opportunities to fabricate novel nanodevices. Filled nanotubes leading to improved catalysts and biosensors are being developed [7] and monoadducts and multiple adducts on C_{60} are finding applications [8]. Therefore, it may be possible to make gears by bonding rigid molecules (gear teeth) onto nanotubes. It may be practical to position molecular teeth in atomically precise positions required for gear design by, say, scanning tunneling microscopy (STM) techniques. Recently, IBM scientists [9] have succeeded in positioning individual molecules at room temperature by purely mechanical means. They used the extremely fine tip of an STM to position organic molecules having a total of 173 atoms and a diameter of 1.5 nm.

Our extensive quantum chemical calculations and molecular simulations support the chemical feasibility of nanotube-based gears [10]. A simple approach is to bond rigid planar benzyne molecules onto a nanotube. The calculations are in agreement with experiment for napthylene and buckyballs (C_{60}) while experimental verification using nanotubes has not been reported. This paper evaluates the nanotube-based gears via molecular dynamics simulation. By studying the rotational dynamics of gears under various conditions, we determine favorable gear working conditions and characterize gear performance.

2. Simulation details

We have chosen Brenner's potential to describe bonded interactions [11]. This potential realistically describes

† To whom correspondence should be addressed. E-mail address: han@nas.nasa.gov

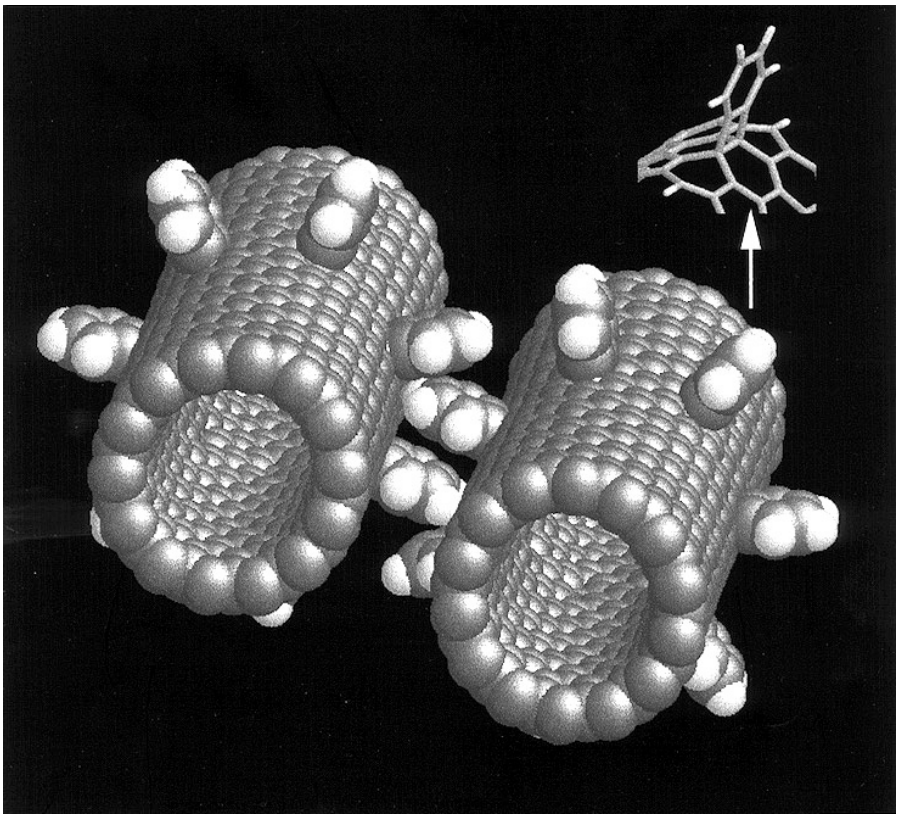

Figure 1. Carbon nanotube-based gears with benzyne teeth.

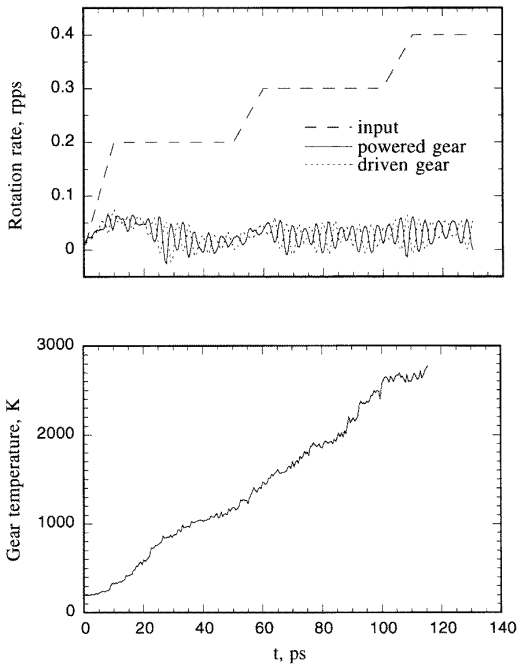

Figure 2. Rotation rate and gear temperature for gear simulation without temperature control.

bonding structure and properties in graphite, diamond materials and small hydrocarbon molecules. In addition, its proper description of bond forming and breaking can be used to observe possible reactive molecular gear failure modes. For intermolecular interactions between different gear atoms, we used and tested several force field potentials: Lennard–Jones (6–12) with parameters derived from fitting graphite and C_{60} experimental data [12] and the Buckingham (exp +6) plus electrostatic interaction terms derived from benzene dimer energy and structure [13]. We carried out molecular mechanics calculations of C_{60}, nanotubes and molecular gears to test these force fields. Minimized energy and C–C bond length are the same as reported values for C_{60} and nanotubes [14]. Energy minimization shows that the nanotube-based gears are stress-relaxed structures, with a slight higher energy than nanotubes ($< 5\%$, depending on length). A detailed comparison with quantum chemistry results is given separately [10]. It shows that Brenner's potential is in good agreement with most of our quantum chemistry results.

Molecular dynamics (MD) simulations were performed on the energy optimized structures. The equations of motion were integrated using a fourth-order predictor-corrector algorithm with a time step of 0.5 fs. The Brendersen's thermostat [15] was used to control the gear's temperature with a time constant of 0.4 ps. This constant was chosen to give a reasonable fluctuation of $\sim$10 K around the assigned temperature. The average temperature had a variation of $\sim$2 K for all the constant temperature simulations. The rotational velocity components in the total atomic velocity were subtracted for evaluation of the thermodynamic temperature. Angular velocity was