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Force and magnetic field sensor based on measurement of tunneling conductance between ends of coaxial carbon nanotubes

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ABSTRACT

The interaction and tunneling conductance between oppositely located ends of coaxial carbon nanotubes are studied by the example of two (11,11) nanotubes with open ends terminated by hydrogen atoms. The Green function formalism is applied to determine the tunneling current through the nanotube ends as a function of the distance between the ends, relative orientation of the nanotubes and voltage applied. The energy favorable configuration of the coaxial nanotubes is obtained by the analysis of their interaction energy at different distances between the nanotube ends and angles of their relative rotation. Using these calculations, a general scheme of the force sensor based on the interaction between ends of coaxial nanotubes is proposed and the relation between the tunneling conductance and measured force is established for the considered nanotubes. The operational characteristics of this device as a magnetic field sensor based on measurements of the magnetic force acting on the coaxial nanotubes filled with magnetic endofullerenes are estimated.

1. Introduction

Unique elastic properties and metallic conductivity of carbon nanotubes allow using the nanotubes as parts of nanoelectromechanical systems (NEMS) (see Refs. [1–3] for a review). The discovery of relative motion of the walls [4] in multiwalled carbon nanotubes (MWNTs) was immediately followed by the idea that NEMS can be based on such a motion [5]. In the last decade, a number of NEMS based on the relative motion of nanotube walls have been implemented experimentally. Among these devices, there are nanomotors in which walls of a MWNT play roles of the shaft and bush driven by an electric field [6–8] or a thermal gradient [9] and memory cells operating on relative sliding of the walls along the nanotube axis [10,11]. A wide set of such NEMS have been also proposed and studied theoretically, including a gigahertz oscillator [12,13], an accelerometer [14,15], a nanothermometer [16], an ultrahigh frequency resonator based on the relative vibrations of the nanotube walls [17], a bolt/nut pair [9,18–20], a nanoactuator in which a force directed along the nanotube axis leads to rotational motion of the walls [21] and a scanning rotational microscope [22].

The characteristics of the memory cells mentioned above [10,11], such as the conductance in the "ON" state, operational frequency, and possibility to use the cells in volatile or non-volatile memory, are determined by interaction and conductance between oppositely located ends of coaxial carbon nanotubes. Thus, theoretical modeling of the interaction and conductance between nanotube ends holds the key to success of these applications. In the present paper, atomistic calculations of the interaction energy between ends of coaxial carbon nanotubes using semi-empirical potentials are accompanied by calculations of the tunneling conductance in the framework of the Green function formalism. The results of these calculations can be used for simulation and comprehensive analysis of operational characteristics of nanotube-based NEMS and nanoelectronic devices. A set of force and mass sensors based on measurements of frequency of string-like

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vibration of carbon nanotubes have been implemented [23–25]. The sensor based on such measurements was proposed to be used to determine magnetic moment of a nanoobject attached to a nanotube [26]. The change of nanotube conductance at nanotube torsion [27] or bending [28] and dependence of the tunneling conductance between nanoobjects at their relative displacement at subangstrom scale [16,29,30] can be used for NEMS elaboration. Particularly a nanothermometer based on measurements of the tunneling conductance between walls of a double-walled carbon nanotube [16] and a nanodynamometer based on measurements of the tunneling conductance between adjacent graphene layers [29,30] have been proposed. In [31] the shielding of external axial constant magnetic field by induced currents in zigzag $(n, 0)$ nanotubes is examined theoretically. Enhancement (paramagnetic response of nanotube for n multiply of 3) or reduction (diamagnetic response of nanotube for n aliquant of 3) of external magnetic field is manifested in induced chemical shifts of NMR signal from molecules encapsulated in nanotube. In principle, the chemical shift of NMR signal allows to estimate the value of external magnetic field. Here we develop a general scheme and operational principles of the force sensor based both on relative motion of carbon nanotubes walls and measurements of the tunneling conductance between their ends.

We also suggest that filling of coaxial nanotubes in the proposed force sensor with magnetic endofullerenes can be used for measurements of magnetic fields. A variety of endofullerenes and nanotubes filled with fullerenes (nanotube peapods), including nanotube peapods filled with magnetic endofullerenes [32–35], can be obtained in macroscopic amounts [36]. It has been also shown that the magnetic moment is greater for magnetic endofullerenes inside carbon nanotubes than for the same magnetic endofullerenes when they are isolated [35]. Recently operational characteristics of the magnetic nanorelay based on bending of the nanotubes filled with the magnetic endofullerenes have been calculated [37]. Here we consider the possibility to determine a magnetic field through measurements of the magnetic force between two coaxial nanotubes filled with the magnetic endofullerenes using the proposed force sensor. Up to now the largest magnetic moment of 21 Bohr magnetons has been observed for $(Ho_3N)@C_{80}$ [38]. The operational characteristics of the magnetic field sensor based on the coaxial (11,11) nanotubes filled with the $(Ho_3N)@C_{80}$ magnetic endofullerenes with the largest observed magnetic moment are calculated.

The paper is organized in the following way. In Section 2, we determine the optimal configuration of the coaxial nanotubes by consideration of the van der Waals interaction between their ends. In Section 3, the results of calculations of electron tunneling current between the ends of coaxial carbon nanotubes as a function of the distance between them and the voltage applied are given. Section 4 is devoted to the general scheme, operational principles and characteristics of the considered system as a force sensor. In Section 5, we discuss the possibility to use this sensor for detection of magnetic fields through measurements of magnetic forces. Our conclusions are summarized in Section 6.

2. Van der Waals interaction calculations

To start consideration of tunneling between coaxial carbon nanotubes we have first determined their energy favorable configuration. Calculations of interaction energy between two coaxial carbon nanotubes (Fig. 1) have been performed using in-house MD–kMC (Molecular Dynamics–kinetic Monte Carlo) code [39]. Two (11,11) single-walled carbon nanotubes of 12.9 Å length with both edges passivated with hydrogen atoms are separately geometrically optimized using the Brenner potential [40] (the binding

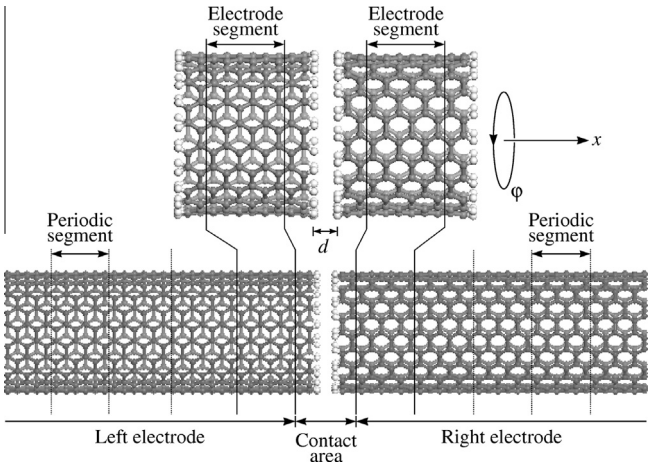

Fig. 1. Atomic model used for calculations of electron transport and van der Waals interaction between coaxial (11,11) carbon nanotubes with the edges terminated by hydrogen atoms. (Below) The system with semi-infinite (11,11) carbon nanotube electrodes for which electron transport calculations are performed. (Above) The finite (11,11) carbon nanotubes used for calculations of the van der Waals interaction and electronic structure of the contact area of the nanotubes and its coupling to the electrodes. The vertical solid lines denote the contact area and segments of the electrodes within the finite model of the nanotube contact. The vertical dotted lines denote periodic segments of the semi-infinite electrodes that are used in the calculations. Carbon and hydrogen atoms are colored in gray and white, respectively. φ is the angle of relative rotation of the nanotubes around the common axis.

energy of the nanotubes and its dependence on relative orientation of the nanotube change by no more than 1% and 2%, respectively, upon increasing the nanotube length twice). Then the walls are considered as rigid, brought together in the coaxial configuration, shifted along the axis and rotated with respect to each other. The interaction between carbon nanotubes is described using the Lennard-Jones 12-6 potential

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad (1)$$

where $\sigma_{CC} = 3.40$ Å, $\sigma_{HH} = 2.60$ Å, and $\sigma_{CH} = 3.00$ Å, $\varepsilon_{CC} = 3.73$ meV, $\varepsilon_{HH} = 0.650$ meV and $\varepsilon_{CH} = 1.56$ meV for carbon–carbon, hydrogen–hydrogen and carbon–hydrogen interactions, respectively [41].

First the global energy minimum for two rigid nanotubes has been found. This energy minimum corresponds to the distance d between the nanotube ends along the nanotube axis of $d_0 = 2.26$ Å and the relative orientation of the nanotubes shown in Fig. 1. The binding energy of the nanotubes is found to be −0.746 eV (Fig. 2b). The energy favorable orientation of the carbon nanotubes corresponds to the case when hydrogen atoms of one of the nanotubes are located in the middle between hydrogen atoms of the neighboring edge of the second nanotube, i.e. at the given distance between the nanotubes, the hydrogen atoms tend to be as far as possible from each other. For the distance between the nanotube ends of $d_0 = 2.26$ Å, the distances between adjacent hydrogen atoms of different nanotubes lie in the range from 2.4 Å to 2.7 Å. There are two such minima per rotational period of the (11,11) nanotubes (Fig. 2a). We denote this relative orientation of the carbon nanotubes as A and the corresponding angles as $\varphi = 0^\circ$, $(360/22)^\circ$, $(360/11)^\circ$, etc.

The dependence of interaction energy of the carbon nanotubes on their relative orientation for the distance between the nanotube ends of $d_0 = 2.26$ Å has two types of maxima (Fig. 2a). The highest maximum C with the relative energy of 0.12 eV corresponds to the configuration in which hydrogen atoms of the neighboring edges of