Nanoelectromechanical systems (NEMS) is a rapidly expanding research field with high potential for applications. Typically, the length scale of these systems is in the nanometer range and there is a strong coupling between the mechanical and electrical degrees of freedom. Key properties of NEMS are high natural frequencies, operation at ultra-low power, and low dissipation. Carbon nanotubes (CNTs) have extraordinary properties that make them ideal building blocks of NEMS. They are light, have very high Young’s modulus and can be elastically deformed without breaking in addition, CNTs have a wide range of electric properties: they can for instance be either semi-conducting or metallic depending on detailed structure.

In this article, we analyze a nanorelay system in which a conducting multi-wall CNT (MWNT) is placed on a terrace in a silicon dioxide substrate and connected to three electrodes. This system has previously been studied by Kinaret et al. who introduced a simple model and discussed the characteristics of the device. In the present work, we focus on the effects of van der Waals and short range forces in the system. We show that the magnitudes of these forces are comparable to those of the elastic and electrostatic forces and that they need to be included in a more realistic model of the system. A brief account on this topic has been presented in Ref. 1. The surface forces alter the system’s behavior, and the characteristics prove to be useful for an application of the relay as a memory element.

We also investigate the dynamic performance of the proposed memory element and estimate its write times. We show that the switching time depend sensitively on dissipative surface processes related to tube-surface interactions when the tube impinges on the drain contact, and analyze this in more detail using a simple model phonon emission. The dissipation associated with this interaction changes the switching time scale of the relay, and consequently, change the typical write time of the proposed memory element.

A schematic picture of the system is presented in Fig. 1. A metallic multi-wall carbon nanotube of length \( L = 50 - 150 \) nm, and step height \( \tilde{h} = 5 - 10 \) nm. By applying a voltage to the gate and/or the drain electrodes, an excess charge \( q \) is induced in the tube. This causes an electrostatic force that deflects the tip of the nanotube towards the drain electrode.

The tube is modeled using classical continuum elasticity theory considering the CNT to be an elastic cantilever with only the lowest vibrational eigenmode excited. Furthermore, we assume that the bending profile of the tube affected by an external force \( F \) is the same as for free oscillations. Then the potential energy of the tube can be expressed in terms of tip deflection \( z \) according to \( V = kx^2/2 \) where the effective spring constant is given by \( k \approx 3EI/L^3 \), where \( I = \pi(D_o^4 - D_i^4)/4 \) is the moment of inertia of the cantilever, and \( E \) is the Young’s modulus, experimentally measured to be of the order of 1 TPa. The equation of motion for the tip of the tube is that of a forced harmonic oscillator with an effective mass given by \( m_{eff} = k/\Omega^2 \approx 3M_{CNT}/(1.875) \) where \( \Omega \) is the lowest vibrational eigenfrequency and \( M_{CNT} \) is the total mass of the CNT-cantilever. In addition, a phenomenological viscous damping \( \gamma_\alpha \dot{z} \) is introduced into the equation of motion. \( \gamma_\alpha \) is estimated from Q-factors from experimental data. Finally we arrive at the equation of motion as:

\[
\gamma_\alpha \frac{d^2z}{dt^2} + k\frac{dz}{dt} + \frac{1}{m_{eff}}V(z) = F(t)
\]
motion

\[ m_{\text{eff}} \ddot{x} = -k x - \gamma_d \dot{x} + F_c + F_{vdW} + F_{sr}, \]

where \( F_c \) is the capacitive force, \( F_{vdW} \) is the van der Waals force, and \( F_{sr} \) are the short range forces due to wave function overlap. These different forces will be discussed in more detail in the next section. The charge dynamics in the tube is governed by

\[ Z \ddot{q} = -q \left( \frac{1}{C_g(x) + C_d(x)} + V_s \right) - V_g \left( \frac{C_g(x)}{C_g(x) + C_d(x)} - ZI_{\text{sd}} \right), \]

where \( V_s \) and \( V_g \) are the electrostatic potentials on the source and the gate, respectively, \( Z \) is the source junction impedance, \( C_g \) and \( C_d \) are the capacitances between the tube and the gate and the drain respectively, and \( I_{\text{sd}} \) is a stochastic tunneling current between the tube and the drain electrode. Due to the much larger tube-gate separation tunneling to the gate is neglected. We choose \( V_d = 0 \).

The tunneling rates of the stochastic tunneling current are calculated using the theory of Coulomb blockade in the presence of an electromagnetic environment. Following Ingold and Nazarov, assuming an ohmic environment and zero temperature, the tunneling rate \( \Gamma \) for a given deflection \( x \) is determined by

\[ \Gamma(x) = \frac{1}{e^2 R_T(x)} \int_0^V (eV - E) P(E) dE, \]

where \( R_T \) is the tunneling resistance and \( V \) is the electrostatic potential difference between the tube and the drain contact (\( V \approx V_g \)). Furthermore, \( P(E) \) is the probability

for energy exchange between the tunneling electron and the environment and is self-consistently determined from

\[ EP(E) = \frac{2Z}{R_K} \int_0^E dE' \left[ 1 + \left( \frac{\pi Z}{R_K} \right)^2 \left( \frac{E - E'}{E_c(x)} \right)^2 \right]^{-1} P(E'), \]

where \( E_c(x) = \frac{e^2}{2C_g(x)} \), where \( C_g(x) = C_d + C_g \) is the total capacitance between the tube and the contacts and \( R_K = 2\pi \hbar/e^2 \approx 25.8 \text{ k\Omega} \) is the von Klitzing constant. The tunneling resistance is approximated by

\[ R_T = R_0 e^{(h-x)}/\lambda, \]

where \( R_0 \) is the tunneling resistance when the tube is in mechanical contact with the electrode, \( \lambda \) is the material dependent tunneling length of the order of 0.5 Å and \( h \) is the tip-contact separation at zero deflection. Note that \( h < h \) since the contact is deposited on top of the substrate.

### III. FORCES

#### A. Electrostatic Force

A numerical solution to the Poisson equation using a finite element method suggests that we can approximate the capacitances of the junctions with a parallel plate capacitor model with an offset. The capacitances between the tube and the gate electrode \( C_g \) and the tube and the drain electrode \( C_d \) are given by

\[ C_d(x) = \frac{C_0}{1 - \frac{25}{h}(1 - C_0/C_h)}, \]

\[ C_g(x) = \frac{2C_0}{1 - \frac{25}{h}(1 - C_0/C_h)}, \]

\[ \text{Figure 1: (a) A schematic picture of the system. One end of a conducting multi-wall carbon nanotube of length } L, \text{ inner diameter } D_i, \text{ outer diameter } D_o \text{ is attached to a source (s) electrode above a step of height } h \text{ in a silicon dioxide substrate. The other end is free to move. The displacement } x \text{ of the nanotube tip is measured towards the substrate. A gate (g) and a drain (d) electrode are placed beneath the tube and are used to control the motion of the tip. (b) An equivalent circuit for the system in Fig. 1(a). The impedance } Z \text{ is ohmic and describes the tube-source coupling. The tube-gate coupling is purely capacitive with the capacitance } C_g(x) \text{ whereas the tube-drain coupling is a tunnel junction with tunneling resistance } R_T(x) \text{ and capacitance } C_d(x). V_{s,g,d} \text{ are the electrostatic potentials on the electrodes and we choose } V_d = 0. \]
where \( C_0 \) is the drain junction capacitance at zero tube deflection, \( C_h \) is the drain junction capacitance when the tube is in mechanical contact with the drain electrode, and \( \kappa = 0.5(3z_f^2 - z_0^2) \) takes into account that the deflection at the tube above the gate is smaller than at the tip. The value of \( C_h \) is estimated from experimental data and \( C_0 \) is calculated for parallel plate capacitors. The resulting capacitive forces are given by

\[
F_c = -\nabla \left( \frac{q_d^2}{2C_d} + \frac{q_s^2}{2C_s} \right),
\]

where \( q_d, q_s \) are the charges on the drain and gate capacitors respectively, \( q_d + q_s = q \), and \( q \) is assumed to be constant during an infinitesimal displacement of the tube.

**B. Van der Waals force**

The origin of the van der Waals (vdW) force is correlation of fluctuating higher order electrostatic moments between two charge distributions. The force is attractive and the interaction energy varies with separation as the inverse sixth power of separation in the range of separations relevant to the nanorelay. The total vdW-energy between the tube and the substrate plus contacts is calculated in a continuum limit. The pairwise sum over the interaction between the individual atoms is transformed into a six-dimensional integral over the volumes of the interacting bodies. In this approximation we can write the vdW-force as

\[
F_{vdW} = -\nabla E_{vdW} = -\nabla \int V_1 \int V_2 \int_{n_1(r_1)}^{n_2(r_2)} dV_1 dV_2 \frac{-C_6}{|r_1 - r_2|^6} n_1 n_2,
\]

where \( V_1 \) is the volume of the tube, \( V_2 \) is the volume of the contacts and substrate, and \( n_1(r_1) \) and \( n_2(r_2) \) are the atom densities in the two bodies. The values of the interaction parameter \( C_6 \) depend on the species of the interacting atoms and is usually stated in terms of the Hamaker constant \( A = \pi^2 n_1 n_2 C_6 \). The Hamaker constant for interaction between graphite-silicon dioxide is given by \( A = 0.07 \text{ aJ} \) and for graphite-metal the corresponding value is 0.6 aJ.

Evaluating the integral in Eq. (9) is time-consuming for an arbitrary geometry. To simplify this, we separate \( E_{vdW} \) in two parts, one contribution from tube-electrode interaction and one from tube-substrate interactions. The substrate is approximated by a semi-infinite plane and the drain electrode is assumed to be cylindrical and infinitely long. Furthermore, we assume that the interaction between the tube and the gate electrode is much smaller than the tube-drain interaction due to the much larger separation. Assuming the MWNT to consist of individual CNTs separated by 3.4 Å, we transform the integral over one-dimension to sum over all individual CNTs in the MWNT. Many of the integrals in (9) can be carried out analytically, leaving either one (for tube-substrate interaction) or three (for tube-electrode interaction) to be evaluated numerically.

**C. Short Range Forces**

The attractive part of the short range force \( F_{att} \) originates from a coupling between the tube and the contact when the electronic wave functions overlap. It can be roughly related to the tunneling conductance \( G_T = 1/R_T \) between the tube and the contact as

\[
F_{att} \propto \sqrt{G}.
\]

A more detailed analysis of the this force is rather complicated but does not change the qualitative features of the system’s behavior. When the core-core separation of the atoms in the tube and in the tip becomes small, however, the wave function overlap increases and we expect a strong repulsion due to the Pauli principle. Taking this repulsive part \( F_{rep} \) to be exponential we model the attractive and the repulsive short range forces by a Morse curve

\[
F_{sr} = F_{att} + F_{rep} = \frac{f }{2\lambda} \sqrt{\epsilon_C \epsilon_T R_K G_0 (e^{-\frac{1}{2}(h-x)} - e^{-\frac{1}{2}(h-x)})},
\]

where \( f \) is a dimensionless shape factor of the order of one, \( \epsilon_T \) and \( \epsilon_C \) are the valence band widths of the tube and the drain electrodes, respectively, and \( G_0 = 1/R_0 \) is the conductance at contact. We define the location of the surface by \( F_{sr} = 0 \). The core-core separation between the atoms in the tube and the drain electrode when the tube is in mechanical contact with the electrode is assumed to be 3 Å. This offset is introduced to prevent the unphysical divergence in the vdW-energy at zero tube-drain electrode separation.

**IV. PHONON EXCITATION**

The only dissipative mechanism in the equation of motion thus far is a viscous damping. Several other dissipative mechanisms are present in a real system. One effect that is important for the device performance is the possibility of phonon excitation in the drain contact when the tube bounces off the surface of the drain electrode. This surface dissipation is importanf for the switching behavior.

**A. Phonon model**

To estimate the dissipation associated with phonon emission we use a simplified classical one dimensional model of the atomic structure. The atomic lattice is modeled as a collection of atoms, each connected to the
Figure 2: The magnitude of the different forces in the system with parameters given in chapter V. The voltages $V_g = 7.5 \text{ V}$ and $V_g = 0.01 \text{ V}$ were used. Close to the contact located at $x = h$ the forces are of the same order while electrostatic and elastic forces dominate far from the surface.

Figure 3: Stability diagram with and without surface forces for the system with parameters given in Chapter V. The curve shows the positions of zero net force on the tube (or local equilibria) as functions of gate voltage (at constant $V_s = 0.01 \text{ V}$) and deflection $x$ (in units of $h$). The large arrows shows the direction of the force on each side of the curves, indicating one local equilibrium to be unstable. The required voltage for pulling the tube to the surface ("pull-in voltage") is given by A ($\approx 6.73 \text{ V}$). In agreement with reference 15 this voltage is not significantly affected by surface forces. A tube at the surface will not leave the surface until the voltage is lower than the "release voltage", B and C in the figure. Note that A > B, C which indicate a hysteretic behavior in the $V_g$-characteristics, a feature significantly enhanced by surface forces.

Figure 4: The remaining kinetic energy of the tube in units of incident kinetic energy as a function of incident velocity. Increasing the incident velocity increases the relative dissipation. The nanotube has an effective mass of $2.1 \cdot 10^{-21} \text{ kg}$ corresponding to the effective mass for the typical system described in chapter V.

other through a harmonic potential, characterized by a spring constant $K$. Assuming linear dispersion relation we obtain the spring constant

$$K = \frac{Mc^2}{a^2},$$

(12)

where $M$ is the mass of the atoms in the chain, $a$ is the equilibrium separation between atoms, and $c$ is the speed of sound in the electrode material. We consider the drain electrode to be made of gold, and thus, we use the lattice constant of gold $a = 407.8 \text{ Å}$, the mass of one gold atom $M = 197 \text{ amu}$, and the sound velocity in gold $c = 2000 \text{ m/s}$.

On the atomic scale the nanotube is a very large object and, thus, the tube will interact with the surface over an extended region while bouncing. We estimate that the impact area of the nanotube corresponds to about 50 gold atoms (an impact area of the order of 2 nm$^2$) in the contact. Instead of considering the motion of each atom in the lattice, we consider the motion of layers of atoms, each layer made up of 50 atoms. The nanotube, characterized by the effective mass $m_{\text{eff}}$, impinges on the model lattice with an initial velocity $v_{\text{in}}$, interacts with the topmost layer through a repulsive force $F_{\text{rep}}$ and bounces. We use a total number of 100 layers, a number chosen such that the boundary conditions at the last layer have only minor importance. The motion of the lattice layers and the nanotube is governed by classical dynamics and the resulting one-dimensional problem is solved numerically.

The one-dimensional model we use does not, e.g., take into account phonons with different polarizations, hence, the model most likely underestimates surface dissipation.
V. RESULTS

A. Effects of Surface Forces

The surface forces introduce constraints on the design parameters. For the operation of the relay it is necessary that

\[-kx + F_x + F_{vdW} + F_{sr} > 0 \quad (13)\]
\[-kx + F_x + F_{vdW} + F_{sr} < 0 \quad (14)\]

in order to both enable pulling the tube to the contact and for the tube to release when the voltage is turned off. In particular, the latter condition is hard to fulfill – a manifestation of the ubiquitous stiction problem in nano-science.

We investigate the behavior of a typical system where Eqs. (13) and (14) are satisfied. The geometrical parameters of this system are tube length \(L = 120 \text{ nm}\), inner tube diameter \(D_i = 2 \text{ nm}\), outer tube diameter \(D_o = 8.8 \text{ nm}\), tube contact separation at zero deflection \(h = 5 \text{ nm}\), relative position of the gate \(z_e = 0.7\), and Young’s modulus \(E = 1 \text{ TPa}\). With these geometrical parameters the effective mass is \(m_{\text{eff}} \approx 2.1 \cdot 10^{-21} \text{ kg}\). Other parameters are source junction impedance \(Z = 8 \text{ k} \Omega\), quality factor of the viscous damping \(Q = 250\), capacitance at zero deflection \(C_0 = 1.3 \cdot 10^{-19} \text{ F}\), and capacitance at contact \(C_h = 5 \cdot 10^{-18} \text{ F}\).

The magnitudes of the forces in a typical system are depicted in Fig. 4 as a function of the deflection of the tube. When the tube tip is near the drain electrode, all forces are comparable, while far from contact the electrostatic and mechanical forces dominate.

The effects of the surface forces can be visualized by means of a stability diagram which shows the positions of zero net force (local equilibria) on the cantilever as a function of gate voltage and deflection. A typical stability curve for the system is given in Fig. 3. A stability diagram with more than one local equilibrium for a specific voltage results in a hysteretic behavior in the IV-characteristics (more than one position of zero net force means that there actually are three such positions, one of which is not stable). This is because the net force is positive to the right of the curve and negative to the left of the curve, so that, when lowering the voltage for a tube in contact with the drain electrode, it will not release until there is no stable position at the surface. Fig. 4 shows that this effect is significantly increased by the surface forces.

The “sticking problem” corresponds to a stable nanotube position for zero voltage at the surface, i.e. failure to satisfy (14). This problem can be alleviated e.g. by choosing stiffer or shorter tubes. This in turn leads to higher voltages needed to satisfy equation (13). With high voltages and small distances, the electric field strengths can be very high. Under these conditions field emission may be important. Simulations show, however, that design parameters can be chosen so that this has a negligible effect.

Figure 5: Step response (gate voltage step \((0 \rightarrow -7.5 \text{ V})\) applied at \(t = 2 \mu\text{s}\)) of the system with parameters given in chapter V without phonon dissipation (elastic bounce) and with surface dissipation (inelastic bounce). The dissipative mechanism reduces the total time of switching by nearly two orders of magnitude. The noise reflects the stochastic nature of the tunneling between the tube and the drain electrode (shot noise).

Figure 6: The IV-characteristics for a typical system with the parameters given in Chapter V has a large hysteresis loop. The arrows indicate up- or down sweep of \(V_g\) (at constant \(V_d = 0.01 \text{ V}\)). The system switches to the conducting state at \(V_g \approx 6.7 \text{ V}\) which agrees well with the expected value deduced from Fig. 3. The reverse transition when lowering the gate voltage takes place at \(V_g \approx 3.1 \text{ V}\) which is slightly larger than the expected value. This small discrepancy is due to small vibrations of the tube and non-adiabatic voltage sweep.
As the incident velocity of the tube increases a larger percentage of energy is transferred from the tube to the substrate. For our particular set of simulation parameters we get a loss function according to Fig. 4. For high incident velocities we get high dissipation whereas for low velocities the relative dissipation gets smaller. This property makes relaxation towards the surface fast even for high initial velocities.

The main effect of exciting phonons in the drain contact is to change the switching dynamics of the relay. Without this dissipative mechanism, relaxation of the tube towards a stationary current carrying state is slow due to the fact that the tube bounces off the contact surface many times before coming to a rest. This time scale is significantly decreased when phonon dissipation is included in the model. A comparison between a simulation showing the response to an applied step gate voltage without dissipation and an equivalent simulation with surface dissipation, depicted in Fig. 5, show that the time scale of switching is decreased by two orders of magnitude. The reverse transition is not affected by including phonon dissipation in the model.

C. Memory Element Application

We have performed numerical simulations of the system described above and the resulting IV_{g}–characteristics at a constant V_{g} = 0.01 V are shown in Fig. 6. The hysteresis is large, which makes a memory element a promising application of the device. In such a memory element the conducting state can be defined as a logical 1 and the non-conducting state as a logical 0. The system is biased at a gate voltage chosen to lie within the hysteresis loop where the system is bistable. The element is written by applying a high/low voltage for a specific write time, T_{w}. The low voltage is typically zero and high voltage is chosen such that the condition (13) is fulfilled. The write times must be long enough to ensure that the correct state is reached, and depend on the chosen write voltages.

We have estimated the write times of the memory element by numerical simulations. Such simulations for the chosen set of parameters are depicted in Fig. 7. The write time for 0 → 1 is approximately 0.8 ns and for 1 → 0 the write time is about 0.02 ns. The difference between these time scales can be explained by comparing the two write processes: When the tube moves from a stationary 1, the tunneling resistance increases exponentially with tube contact separation and the current will stop soon after the voltage is switched off. In the 0 → 1 transition the tube bends relatively quickly to the drain electrode, but tends to bounce off the surface. The kinetic energy of the mechanical motion must be dissipated before the tube relaxes toward the stationary 1-state. This relaxation is enhanced due to phonon dissipation in the drain, but we cannot expect it to remove the asymmetry completely. The time scale corresponding to the 0 → 1 transition sets the limit for maximum operating frequency, approximately 1 GHz for the parameters we have used.

VI. CONCLUSIONS

We have incorporated short range and vdW-forces into a model of a three terminal nanorelay. The main effect of these forces is to increase the hysteresis in the IV_{g}–characteristics making a memory element a promising application of the relay. We have investigated the switching characteristics for such a memory element and conclude that the write dynamics is limited by the 0 → 1 transition. The transition dynamics of the 0 → 1 transition depends to a great extent on the dissipative surface processes when the tube bounces, which reduce the transition time by two orders of magnitude, whereas the 1 → 0 transition is unaffected by such processes.
Acknowledgments

We would like to thank the Swedish Foundation for Strategic Research for funding this project through the CARAMEL (Carbon Allotropes for Microelectronics) consortium and the framework program on CMOS-integrated carbon-based nanoelectromechanical systems. One of the authors (T.N.) acknowledges financial support from the Swedish research council (VR).

1. M. Roukes, Phys. World 25, 2001; Opening lecture, 2000, Solid State Sensor and Actuator Workshop, Hilton Head, SC, 6/4/2000, published in Technical Digest of the 2000 Solid State Sensor and Actuator Workshop.
2. E. W. Wong, P. E. Sheehan, and C. M. Lieber, Science 277, 1971 (1997).
3. B. I. Yakobson, C. J. Brabec, and J. Bernholc, Phys. Rev. Lett. 76, 2511 (1996).
4. R. Saito, G. Dresselhaus, and M. Dresselhaus, Physical Properties of Carbon Nanotubes (Imperial College, London, 1998).
5. J. M. Kinaret, T. Nord, and S. Viefers, Appl. Phys. Lett. 82, 1287 (2003).
6. M. Jonsson, M.Sc. thesis, Chalmers University of Technology, (2003).
7. M. Jonsson, T. Nord, S. Viefers, and J. M. Kinaret, in Proc. of the Electrochemical Society: Fullerenes vol. 13 - Fullerenes and Nanotubes: The Building Blocks of Next Generation Nanodevices, editors D. M. Guildi, P. V. Kamat, and F. D. Souza (Electrochemical Society, Pennington, 2003)
8. L. D. Landau and E. M. Lifshitz, Theory of Elasticity (Pergamon, Oxford, 1986).
9. M. M. Treacy, T. W. Ebbesen, and J. M. Gibson, Nature (London) 381, 678 (1996).
10. E. P. Wong, P. E. Sheehan, and C. M. Lieber, Science 277, 1971 (1997).
11. P. Poncharal, Z. L. Wang, D. Ugarte, and W. A. de Heer, Science 283, 1513 (1999).
12. G. L. Ingold and Y. V. Nazarov, in Single Charge Tunneling, NATO ASI Series B:Physics, edited by M. H. Devoret and H. Grabert (Plenum, New York, 1992), p. 21-107.
13. T. Johansson, M.Sc. thesis, Chalmers University of Technology (2001).
14. R. Tarkiainen, M. Ahlskog, J. Penttilä, L. Roschier, P. Hakonen, M. Paalanen and E. Sonin, Phys. Rev. B 64, 195412 (2001).
15. L. W. Bruch, M. W. Cole, and E. Zaremba, Physical Adsorption: Forces and Phenomena. (Oxford, Clarendon, 1997).
16. M. Dequesnes, S. V. Rotkin, and N. R. Ahru, Nanotechnology 13, 120 (2002).
17. F. O Goodman and N. Garcia, Phys. Rev. B 43, 4728 (1991).
18. C. J. Chen, J. Phys.: Cond. Mat. 3, 1227 (1991).
19. J. C. Slater, Quantum Theory of Molecules and Solids, vol 1 (McGraw-Hill, New York, 1963).
20. S. Ciracci, E. Tekman, A. Baratoff, and I. P. Batra, Phys. Rev. B 46, 10411 (1992).
21. N. W. Ashcroft, N.D. Mermin, Solid State Physics (Harcourt, Orlando, 1976).
22. S. Axelson, private communication.
23. This macroscopic treatment can also be regarded as a first order Taylor expansion of $1/C(x)$. 