Current correlation functions for chemical sensors based on DNA decorated carbon nanotube

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Abstract

The current characteristics of DNA decorated carbon nanotubes for different gas odors are studied. A simple model of charge transfer between the Gas-DNA-base complex and single wall carbon nanotube (SWCN) is proposed to explain the current response for different odors. The autocorrelation and two-point correlation functions are calculated for the current sensitivity curves. These correlation functions together with the current characteristics form finger-prints for detection of the odor and DNA sequence.

Key words: Carbon nanotube; DNA; Correlation functions; Chemical sensor; Sequence detector

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1 Introduction

The discovery of carbon nanotubes (CNTs) [1] has generated a tremendous amount of interest and activity in basic research and applied technologies. The unique properties of CNTs make them a potentially ideal material for molecular sensing. The simplest nanotube is a single layer of graphite rolled into a seamless cylinder and is called the single wall carbon nanotube (SWCN) having diameters ranging from 1-2 nm [2]. This unique structure results in electronic and chemical properties that are ideal for the direct electronic detection of chemical vapors [3]. The electronic properties of CNTs can be altered by modifying their parent structure [4] and this can be done by doping them with certain molecules or polymers [5,6,7,8,9,10,11,12,13,14,15]. It is found that the conductance of SWCNs changes in response to exposure to certain molecules that undergo charge transfer upon adsorption [5,6,7,8,9,10,11,12,13,14,15]. In particular, CNTs can be functionalized with single stranded deoxyribonucleic acid (ss-DNA) or DNA nucleoside [4,16,17,18,19,20]. Functionalization of CNTs with DNA offers interesting prospects in different fields including detection of chemical vapors, solubilization in aqueous media, and nucleic acid sensing [4,17,18,19,20].

This work presents a theoretical understanding of the current characteristics of gas flow over DNA decorated CNTs [17]. The article [17] studies the nanoscale chemical sensors, with ss-DNA for chemical recognition and single walled carbon nanotube field effect transistors (SWCN-FETs) for electronic readout. The composites, SWCNs coated with ss-DNA, respond to various gas odors that do not respond or cause a detectable conductivity change in the bare devices (without DNA). As a result of functionalization of SWCNs with DNA
a change in the current is observed for each gas odor.

These findings motivated us to analyze the ss-DNA-Gas/SWCN complex system and to understand the reason for the observed change in the current. Our analysis gives two main results: the first is the proposal of a simple phenomenological model based on charge transfer between the Gas-DNA-base complex and the SWCN, and the second is the calculation of the correlation functions for the current characteristic curves of Ref. [17]. We find that the current fluctuations (correlation functions) together with the current characteristics form finger-prints for detection of the odor. More importantly the characteristic pattern of the DNA sequence is captured in these current correlation functions. Hence these gas flow sensors may also be used as sequence detectors for DNA where the pattern of correlation functions may be used as a benchmark for the particular chemical signal encoded in a DNA sequence.

2 Experimental details

SWCNs were synthesized by catalytic chemical vapor deposition (CVD) of methane (2.50 sLm) at 900° C on a SiO₂/Si substrate using iron salt catalyst (Fe(NO₃)₃·9H₂O dissolved in isopropyl alcohol) [17]. Hydrogen (0.320 sLm) and argon (0.600 sLm) are allowed to flow through the furnace throughout the heating and growth process. FETs were fabricated with Cr/Au source and drain electrodes using e-beam lithography and the degenerately doped Si substrate used as a backgate [17,18,19]. The resistance of the FETs was 100 – 500 kΩ [19] in the “ON” state.

1 Standard liters per minute.
The two ss-DNA sequences chosen in the experiment [17] are:

Sequence 1: 5′ GAG TCT GTG GAG GAG GTA GTC 3′

Sequence 2: 5′ CTT CTG TCT TGA TGT TTG TCA AAC 3′.

These oligonucleotides were diluted in distilled water to make a stock solution of 658µg/ml (sequence 1) and 728µg/ml (sequence 2). First the odor responses of bare devices were measured, and then the devices were functionalized with a particular ss-DNA sequence by applying a 500µm diameter drop of the solution to the device for 45 min and then dried in a nitrogen stream [17,18,19].

The adsorption of ss-DNA on SWCNs was characterized by Atomic Force Microscopy (AFM). The AFM images [17,18,19] of the same SWCN before and after the application of DNA show a clear increase in the tube diameter from $5.4 \pm 0.1$ nm to $7.2 \pm 0.2$ nm, indicating formation of a nanoscale layer of ss-DNA on the SWCN surface [17,18,19]. Functionalization of SWCNs with ss-DNA caused the threshold value of the gate voltage $V_g$ to decrease by 3-4 V for measurable conduction and this corresponds to a decrease in the hole density [17,18,19].

The sensor response for five different odors Methanol, Propionic acid (PA), Trimethylamine (TMA), 2, 6 Dinitrotoluene (DNT) and Dimethyl methylphosphonate (DMMP) was studied. Here the focus was on odor induced changes in the current measured with bias voltage $V_b = 100$ mV and $V_g = 0$ V [17]. In this experiment, gas and then air is alternately exposed to the device each for

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2 The mentioned diameter is most likely for a small bundle of nanotubes [19] as the CVD process used in Refs. [17-19] tends to produce nanotubes with a diameter from 1-2 nm.
50 seconds. The experiment is repeated for multiple odor exposures \[17\].

The bare and polymer coated SWCNs respond to various gases \[3,5,6,7,8,9,10,11,12,13,14,15\] but some chemical species interact weakly or not at all with the bare SWCNs \[17,18,19\]. For molecular sensing, it is necessary that the chemical species get adsorbed on the device properly. When SWCNs are coated with DNA the bases bind to SWCNs through vdW forces and by forces due to their mutual polarization \[16,20\]. We propose that the chemical species get adsorbed on SWCNs through vdW forces and/or mutual polarization between the chemical species and DNA-SWCN complex (as in Refs. \[16,20\]), Fig. 1. Hence the DNA increases the binding affinity of the molecular species (odors) to the device. The model described below is a phenomenological model. The building of a microscopic (tight binding) model of CNTs is an important task and needs future work.

3 Model

Here we propose a model to explain the sensor response \[17\]. The model consists of a FET in which a p-type SWCN acts as an electronic wire between two metal electrodes with an ss-DNA sequence on it. For clarity of exposition the model illustrated in Fig. 2 has a simpler geometry than the experiment.

**DMMP and 2,6 DNT**: The current response of the bare device is less than the experimental sensitivity \(\Delta I/I \sim 1\%\); where I is the source-drain current) when exposed to DMMP with estimated concentration 25 ppm \[17\]. After coating the same device with ss-DNA sequence 2, exposure to DMMP gives a slight change (decrease) in the current, that is, the sensitivity of the device
is $\Delta I/I = -7\%$ [17]. Due to the application of ss-DNA layer, the binding affinity of DMMP to the device increases through vdW forces and/or mutual polarization [20], this results in an increase in sensor response. The fluctuations in the current response are due to the structure of DNA sequence.

To explain the adsorption of ss-DNA on SWCNs and sensor response mechanism molecular dynamics simulations were done in [18][19]. Another mechanism which needs to be modified to include the effect of the DNA can be a pulsating asymmetrical ratchet model used to describe the flow induced voltage (current)[21]. This may be a future work. Here we propose a simpler mechanism which includes the DNA to describe the current characteristics.

The DNA bases interact with the SWCN in the same way as described in Ref.[20]. The interaction of DMMP with DNA-bases through vdW forces and/or mutual polarization [20] causes charge redistribution and changes the polarization between the DNA and the SWCN leading to a net charge transfer from the Gas-DNA-base complex to the SWCN. These charges are some combinations of $\alpha, \beta, \gamma$ and $\delta$ negative ions which are arbitrary fractional charges transferred by each Gas-DNA-base complex and depend on the DNA sequence and odor. The net charge transfer causes the Fermi level of the SWCN to shift away from the valence band [5], which results in hole depletion of the p-type SWCN-FET sensor and reduces the current. Note that the charge transfer from the Gas-DNA-base complex to the SWCN is larger than the charge transfer from DNA-base to the SWCN as well as from SWCN to the Air-DNA-base complex.

This process continues till all DMMP molecules interact with the full DNA sequence causing a net charge transfer which leads to a minimum value of
the current. A similar mechanism occurs for multiple exposures of the same odor and we get the same minimum value of the current. Thus for each odor exposure the pattern repeats itself indicating the stability of the sensor.

For the next 50 seconds, when air is exposed to the device it replaces the gas molecules as shown in Fig. 2 and interacts with the SWCN through DNA. This causes a net charge transfer from the SWCN to oxygen [11] which shifts the Fermi level closer to the valence band. This increases the hole concentration and enhances the current. This process continues until the maximum value of the current \( I = I_0 \) is reached, where \( I_0 \) is the source-drain current when exposed to air (no odor) [17]. For DNT (40 ppm) the explanation is the same and the sensitivity of the device is \( \Delta I/I = -14\% \) with sequence 1 [17].

**TMA**: The bare device responds to TMA (20000 ppm) [17], because it interacts with the SWCN through vdW forces and/or mutual polarization [20]. The negative charge transfer from TMA to the SWCN neutralizes the holes and reduces the carrier concentration of the sensor and there is a decrease in the current. The observed sensitivity is \( \Delta I/I = -10\% \). After the application of DNA sequence 2 the response is tripled, \( \Delta I/I = -30\% \) [17]. The polarization between the SWCN and TMA-DNA-base complex causes charge transfer from the TMA-DNA-base complex to the SWCN. There is an additional charge transfer due to direct interaction of TMA with the SWCN. Both processes cause a net charge transfer which is far greater than the charge transfer before the application of DNA. On air exposure the current increases and reaches a maximum value \( (I = I_0) \).

**PA**: The sensor response to PA (150 ppm) differs in sign and magnitude from the response to other odors [17]. The interaction of PA with DNA sequence
1 causes a net charge transfer from SWCN to the Gas-DNA-base complex therefore increases the hole concentration and the current response. In this case the sensitivity is $\Delta I/I = +17\%$ \cite{17}. On air exposure the current decreases and reaches a minimum value $I_0$ (maximum for other odors) as the charge transfer from SWCN to the Air-DNA-base complex is small compared to the charge transfer to the PA-DNA-base complex.

*Methanol*: The bare device does not respond to Methanol (4000 ppm). Exposure to Methanol gives $\Delta I/I = -12\%$ with sequence 1 and $\Delta I/I = -20\%$ with sequence 2, \cite{17}. The explanation for the sensor response is the same as given for other odors except PA.

The important aspects of investigation of a variety of sensors are their sensitivity, selectivity, and stability \cite{22}. The above explanation shows how functionalization of SWCNs with ss-DNA is helpful in increasing the sensitivity of the ss-DNA/SWCN-FETs by increasing the binding affinity of the gas molecules to the devices as the bare devices do not respond to these odors except TMA. Table 1 of Ref. \cite{17} shows measured responses of 5-10 devices to gas odors. The interaction of different odors with SWCNs gives different charge transfers leading to distinct patterns of the current characteristics for each odor. This indicates selective recognition of each odor by the ss-DNA/SWCN-FET sensors.

For each odor a constant sensor response is maintained without any need for sensor refreshing through at least 50 gas exposure cycles \cite{17}. The sensor response and recovery time remained the same to within 5%. The variation in odor responses for different devices is small e.g. the sensitivity variation for TMA (sequence 2) is $\Delta I/I = -30 \pm 2\%$ measured with 5-10 devices \cite{17}. This
indicates excellent reproducibility and hence the stability of the sensors.

If the device is exposed to a mixture of gases then the resulting current characteristics will be different from the characteristics observed for each individual gas odor. This is because the sensing material does not respond to a particular odor only, but to a mixture of gas odors. In this case it is difficult to distinguish different odors from the resulting characteristics. This indicates that the selectivity of a sensor gets affected by a mixture of gases.

4 Explanation for the difference in the odor response characteristics of the sensors for two different sequences

We observe, in the Table 1 [17], that there is a larger decrease in the current when TMA/Methanol interacts with DNA sequence 2 than with sequence 1. This indicates that the net charge transfer from the Gas-DNA-base complex to the SWCN is more when TMA/Methanol interacts with sequence 2. We give here a simple explanation using the model, Fig. 2.

When TMA/Methanol interacts with DNA sequence 1 with 21 bases, which consists of 5 Thymine, 10 Guanine, 2 Cytosine and 4 Adenine, each Gas-DNA-base complex gives $\alpha$, $\beta$, $\gamma$ & $\delta$ negative ions that causes a net charge transfer from the Gas-DNA-base complex to the SWCN. Similarly when TMA/Methanol interacts with sequence 2 with 24 bases, which consists of 11T’s, 4G’s, 5C’s & 4A’s, the Gas-DNA-Thymine complex gives $6\alpha^-$ ions more than the value of $\alpha^-$ ions we get with sequence 1, whereas Gas-DNA-Guanine complex gives $6\beta^-$ ions less than sequence 1, Gas-DNA-Cytosine complex gives $3\gamma^-$ ions more than sequence 1 and Gas-DNA-Adenine complex gives $4\delta^-$ ions, which
is the same as in sequence 1. We propose that when TMA/Methanol interacts with sequence 1 (2), the net charge transfer is dominated by transfer of $\alpha^-$ ions (the value of $\alpha > \beta, \gamma, \delta$) which is more for sequence 2 than sequence 1 (because sequence 2 has 11T’s, but sequence 1 has only 5T’s each giving $\alpha^-$ ions). Hence for TMA/Methanol, the current decreases and confirms the result shown in Table 1 [17]. The value of $\alpha^-$ ions is different for TMA and Methanol because both have different current responses. For TMA the decrease in the current is large because of an additional charge transfer due to direct interaction of TMA with the SWCN.

On the other hand, there is increase in the current when DMMP/DNT interacts with sequence 2 as compared with sequence 1. This indicates that the net charge transfer from the Gas-DNA-base complex to the SWCN is increased as we go from sequence 2 to 1. For DMMP/DNT the net charge transfer is dominated by transfer of $\beta^-$ ions (with $\beta > \alpha, \gamma, \delta$) which is small for sequence 2 as compared with sequence 1. The interaction of DMMP/DNT with 10G’s of sequence 1 causes the Gas-DNA-Guanine complex to transfer more $\beta^-$ ions than the $\beta^-$ ions transferred by the interaction with sequence 2 (with 4G’s).

For PA there is decrease in the current when PA interacts with sequence 2 than when it interacts with sequence 1. This shows that the net charge transfer from SWCN to the Gas-DNA-base complex is low. Again the net charge transfer is dominated by transfer of $\beta^-$ ions ($\beta > \alpha, \gamma, \delta$). Hence we see that the odor response characteristics of these sensors are specific to the ss-DNA sequences.

It follows from the model that two distinct sequences with the same number of bases but different order of the bases will give the same minimum value of the current with different current characteristics (active part).
5 Results

5.1 Autocorrelation function

The expression for the autocorrelation function is

\[ P_k = \frac{\frac{1}{N} \sum_{t=k}^{N-1} (I(t) - \bar{I})(I(t + k) - \bar{I})}{\frac{1}{N} \sum_{t=0}^{N-1} (I(t) - \bar{I})^2} \]  

(1)

where \( I(t) = I(t)/I_0 \) is the normalized source-drain current at time \( t \) with \( I_0 \) the value of the current without odor, and \( \bar{I} = \frac{1}{N} \sum_{t=0}^{N-1} I(t) \) is the mean of the current over the time interval \( 0 \leq t \leq (N-1) \). \( N \) is the total number of observations and \( k = 0, 1, 2, 3.. \) is the time lag.

Data analytical methods used in the calculation of the autocorrelation function may be helpful in realizing the sensitivity and selectivity of a sensor. The autocorrelation function is a pattern recognition measure that is useful for finding the repeating patterns in a signal and for detecting long range correlations. The autocorrelation function is a correlation of a data set with itself: the correlation is between two values of the same variable at time \( t \) and \( t + k \) averaged over the whole signal. In the current characteristics [17] the pattern for both gas and air repeats itself. In the calculation we divide the complete pattern [17] into different segments for the exposure time when gas replaces air Figs. 3 (a), (b) and when air replaces gas Figs. 3 (c), (d). For each data segment we calculate the autocorrelation function then we take the average of all the segments and plot the averaged data with respect to time lag, Fig. 3.

We observe that the autocorrelation function is different for different odors
and it is different for both air and odors. The autocorrelation function for air has some structure and is different from the function for randomly generated numbers. The autocorrelation function for odor together with air form a distinct pattern of the Gas/Air-DNA-SWCN system. Note that the autocorrelation function for Methanol with sequence 2, Figs. 3 (a), (c) is different from Methanol with sequence 1, Figs. 3 (b), (d). This shows that the autocorrelation function varies for the same odor with different DNA sequences. Hence the autocorrelation function gives distinct patterns of odor sensitivity indicating the selectivity of a sensor to a particular target odor. Taking logarithm (decade) of the autocorrelation function for Methanol with sequence 1 & 2 and plotting it with respect to time lag we get different slopes for both gas and air, Fig. 4. The different slopes indicate that the autocorrelation function is sensitive to the DNA sequence and strengthens the results found in Fig. 3. The small differences in the slopes show high sensitivity of the sensor. For other odors also we find different slopes indicating the ability of ss-DNA/SWCN-FET sensors to detect minor changes in the current response for different odors.

Our aim in calculating the autocorrelation function is to get a pattern of close points for different odors and sequences, which may relate the ss-DNA sequence with the sensor response. This long range autocorrelation function is sensitive to the full DNA sequence. Using the data from the current characteristics [17] we calculate the autocorrelation function using equation 1.

5.2 **Two-point correlation function**

Let us define the two-point correlation function $G(t)$ for the current as
\[ G(t) = \frac{1}{\tau} \sum_{i=1}^{\tau} I_i(t) I_i(t + \delta t) - \left( \frac{1}{\tau} \sum_{i=1}^{\tau} I_i(t) \right)^2 \]  

(2)

where \( I_i(t) = I_i(t)/I_0 \) is the normalized source-drain current in the \( i^{th} \) gas/air exposure cycle, \( \delta t = 1 \) s and \( \tau \) is the total number of exposure cycles.

Figs. 5 & 6 show the results of this calculation for different odors and DNA sequences upon odor and air exposures. Though there are a lot of fluctuations in the two-point correlation we still observe distinct patterns for the different odors and sequences. This indicates selective recognition of each odor by the sensors. Table 1 shows that the values of correlation function \( G(t) \) upon different odor and air exposures lie in different ranges.

Note the distinct patterns for Methanol with sequence 2 and 1, Figs. 5 (c), (f) and 6 (c), (f). This shows that the Figs. 5 and 6 may be used along with the Fig. 3 to identify the odor and DNA sequence.

6 Discussion and Conclusion

We studied the experiment [17] which involves a change in sensor current upon odor exposure relative to the level measured when the sample is exposed to clean air. The sensor response curves [17] show that the bare SWCN-FET device does not respond to any odor except TMA. We propose that the odors can interact with the SWCN through ss-DNA and the interaction could be the vdw forces and/or mutual polarization [16,20] between the odors and DNA-SWCN. The model (Fig. 2) explains that the interaction between the gas and DNA causes charge redistribution and changes the polarization between the DNA and the SWCN leading to a net charge transfer from the Gas-DNA-base
complex to the SWCN and vice-versa for PA. This is responsible for the sensor response.

For PA, the gas molecules interact with the full DNA sequence before completion of the exposure time (let this time be $t_c$) therefore we find a positive value of the current which remains constant throughout the odor exposure after $t_c$. This shows flatness (saturation) in the pattern of the current characteristics. For methanol with sequence 1 a similar flatness is observed for the same reason.

In experiment [17] we find that to maintain a constant sensor response the odor concentration should be constant. Usually, e.g. in Ref. [9], the sensor response is linear for different concentrations but in experiment [17] this is not observed as the current is a function of time for a fixed concentration. To detect the sensor response the odor concentration and flow rates should be enough to cause charge transfer which is necessary for the sensing material to sense the target odor and should be such that the molecules interact with the full DNA sequence to get the repeated pattern. If the concentration is very low and not enough to cause charge transfer then no response will be observed. If the concentration is low but enough to cause charge transfer, the gas will not occupy the full DNA sequence and the pattern will not repeat itself. If the concentration is higher than required to occupy the full DNA sequence then flatness will occur which limits the characteristic part (active region) of the pattern.

In summary, we have explained the difference in the odor response characteristics of the sensors for two different sequences using the model and calculated the correlation functions indicating that CNTs can be used as chemical sen-
sors as well as sequence detectors. We find from Figs. 3, 5 and 6 that the fluctuations in the current of CNTs are more sensitive to the adsorption of certain types of gases. The correlation plots of ss-DNA/SWCN-FET sensors are different for different odors. Here the autocorrelation function clearly shows that the Methanol with sequence 2 is different from Methanol with sequence 1, Fig. 3. The slopes for Methanol and air with sequence 1 (2) are different (Fig. 4) indicating that the autocorrelation function is sensitive to the DNA sequences and also show selectivity and sensitivity of the sensor. The patterns for the two-point correlators Figs. 5, 6 also show characteristic features of the DNA sequence and odor used. These figures may also be used along with the autocorrelation figures to identify the odor and DNA sequences. The two-point current correlation function $G(t)$ has a universal part and a non-universal (noise) part in mesoscopic systems [23]. The correlators that we have calculated here may also have this structure. We are in the process of trying to understand the physical meaning of these correlation functions for the ss-DNA-Gas/SWCN complex systems in the context of the tight binding model of CNTs.

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Fig. 1. Schematic view of attachment of an adenine base of the ss-DNA sequence 2 and a DMMP molecule on the SWCN through vdW forces or mutual polarization.
Fig. 2. A phenomenological model. The brown and purple balls indicate the gas and air, respectively.
Fig. 3. The autocorrelation function $< P_k >$ versus time lag $k$(sec) for (a) DMMP + sequence 2, DNT + sequence 1 and Methanol + sequence 2 upon gas exposure (b) TMA + sequence 2, PA + sequence 1 and Methanol + sequence 1 upon gas exposure (c) DMMP + sequence 2, DNT + sequence 1 and Methanol + sequence 2 upon air exposure (d) TMA + sequence 2, PA + sequence 1 and Methanol + sequence 1 upon air exposure. These plots distinguish between different odors and DNA sequences.
Fig. 4. The decade logarithm of autocorrelation function ($y = \log<P_k>$) versus time lag ($x = k(\text{sec})$) up to 5 seconds for (a) Methanol + sequence 1 upon gas exposure (b) Methanol + sequence 1 upon air exposure (c) Methanol + sequence 2 upon gas exposure (d) Methanol + sequence 2 upon air exposure. Different slopes indicate that the autocorrelation function is sensitive to the DNA sequence for methanol and the differences in the slopes show sensitivity of the sensor.
Fig. 5. The two-point correlation function $G(t)$ versus time(sec) upon gas exposure for (a) DMMP + sequence 2 (b) DNT + sequence 1 (c) Methanol + sequence 2 (d) TMA + sequence 2 (e) PA + sequence 1 (f) Methanol + sequence 1. This indicates that the fluctuations in the current of CNTs are more sensitive to the adsorption of certain types of gases and DNA sequences.
Fig. 6. The two-point correlation function $G(t)$ versus time(sec) upon air exposure for (a) DMMP + sequence 2 (b) DNT + sequence 1 (c) Methanol + sequence 2 (d) TMA + sequence 2 (e) PA + sequence 1 (f) Methanol + sequence 1. This indicates that the fluctuations in the current of CNTs are more sensitive to the adsorption of certain types of gases and DNA sequences.
Table 1

Range of values of the two-point correlation function $G(t)$ upon odor and air exposures

| Odors & sequence | $G(t) (Odor)$          | $G(t) (Air)$          |
|------------------|------------------------|-----------------------|
| DMMP with sequence 2 | 0.009244 to -0.01888 | 0.016544 to -0.0119   |
| DNT with sequence 1  | 0.032467 to -0.04671 | 0.042489 to -0.05728 |
| Methanol with sequence 2 | 0.037275 to -0.08255 | 0.044994 to -0.03406 |
| TMA with sequence 2   | 0.0092 to -0.02313    | 0.01405 to -0.00718   |
| PA with sequence 1     | 0.064194 to -0.02065 | 0.0246 to -0.02723    |
| Methanol with sequence 1 | 0.01355 to -0.0306   | 0.0203 to -0.01253    |