Coupled NEGF-PSO method for maximizing the current ratio of CNTFETs based on oxide thickness optimization

Amin Ghasemi Nejad Raeini1 · Zoheir Kordrostami1 · Samaneh Hamedi1

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Abstract
A method for designing carbon nanotube field-effect transistors (CNTFETs) with optimized oxide thickness is proposed herein. The optimum oxide thickness that provides the maximum current ratio (on/off ratio) is calculated for each design. The effect of oxide thickness on the on/off ratio is investigated by treating it as the independent variable and calculating the on-state and off-state currents. Particle swarm optimization is used to determine the exact optimum oxide thickness to achieve the maximum current ratio, which is one of the most important parameters in switching applications. The optimum insulator thickness is calculated for CNTFETs with different chiral vectors, insulator types, channel lengths and source/drain doping levels. For further study of the CNTFETs, performance parameters including cutoff frequency and transconductance of the devices are also calculated and investigated. The results show that CNTFET designers should select the oxide thickness very carefully, not simply based on reported values in other works. Each design requires its own optimum oxide thickness which provides the maximum on/off current ratio only for that design.

Keywords Optimization · CNTFET · Current ratio · Oxide thickness · PSO algorithm

1 Introduction
Because of the unique physical and electrical properties of carbon nanotubes (CNTs), they have garnered much attention as electronic material in molecular and nanoscale electronic devices [1–3]. The simple and well-defined structure of single-walled CNTs has encouraged their investigation in both theoretical and experimental studies [4, 5]. The electrical and physical properties of CNTs have been studied extensively in the literature [4]. The use of CNTs as an alternative channel material in metal–oxide–semiconductor field-effect transistors (MOSFETs) has led to greater current density and modified short-channel effects. These are all significant factors that improve the performance of nanoscale FETs [6, 7]. Also, enhanced carrier mobility in CNTs has resulted in higher current density and operating frequency in carbon nanotube FETs (CNTFETs).

Performance optimization of CNTFETs has been an active area of study for some time [8–10]. As for the gate contact, different insulator types and thicknesses have been used in previous works [5–13]. Changes in insulator thickness directly affect the charge transport and energy band in the channel. Thus the insulator thickness can be used as a critical parameter to modify the device characteristics [6].

Various methods for improving the current ratio of conventional CNTFETs and Schottky barrier CNTFETs (SB-CNTFETs) have been reported [6, 12, 13], in which high current ratios have been achieved by tuning the gate insulator parameters at different temperatures. Finding the optimum insulator thickness is a very important research challenge. Many works in the literature have neglected this and have not used optimum insulator thicknesses. In studies by Shirazi and Mirzakuchaki [11] and Raeini et al. [12], tuned gate insulator thicknesses were obtained, but it cannot be claimed that these values were the optimum values, because an optimization algorithm was not used. In most of the works on CNTFET designs, the value of oxide thickness is selected based on previously reported values. Among the works that discuss the effect of oxide thickness on device performance, almost all check only discrete values of oxide thickness and then conclude what the best thickness is. In this paper, we have used two methods to determine the best oxide thickness: (1) changing the values of the oxide thickness (discrete...
values) and calculating their corresponding on/off current ratios, and (2) using the particle swarm optimization (PSO) algorithm with the ability to find the exact value of oxide thickness to achieve the maximum on/off current ratio.

In this paper, we propose using PSO for tuning the gate insulator thickness with the goal of achieving the maximum on/off current ratio. This is an important parameter of FETs and characterizes the difference between the off current and the on current. The current ratio is the figure of merit for achieving better performance, and greater $I_{on}$ and lower leakage current ($I_{off}$) for MOS transistors.

The numerical simulation is based on the Poisson equations and self-consistent solution of the two-dimensional Green’s function [14, 15]. The optimum oxide thicknesses were calculated for CNTFETs with different CNT chiralities, oxide materials, channel lengths and source/drain doping concentrations. The objective of the optimization is to obtain the maximum current (on/off) ratio.

The proposed structures were designed based on the PSO outputs (optimum gate oxide thickness) which provide the highest possible on/off ratios. The characteristics of the proposed designs are compared with each other. Finally, based on the designs and the comparisons, the best structures with superior performance are introduced. The new structures have optimum current ratios and very high cutoff frequencies and transconductance values.

The rest of the paper is organized as follows: A brief review of the PSO algorithm is discussed in Sect. 2. The methodology for the simulation of the CNTFET is discussed in Sect. 3. In Sect. 4, the results of the PSO algorithm (optimum oxide thicknesses) are presented, and the paper is concluded in Sect. 5.

2 Particle swarm optimization method

PSO algorithms are population-based metaheuristic algorithms inspired by nature, originally introduced and developed by Kennedy, Eberhart and Shi [15–18]. These algorithms imitate the behavior of schools of fish and flocks of birds. The PSO algorithm is designed to iteratively search for the optimum solution according to a featured measure starting from a randomly distributed set of particles [15]. Based on interparticle connections and the movement of particles around the search space utilizing a set of simple mathematical equations, the solution is optimized. These mathematical statements, in basic and simplest form, guide the movement of any particle toward its best experienced status and the swarm’s best status, along with some random disorder [15]. PSO is generally utilized as an optimization method and has its roots in computer animation technology and image presentation, where Reeves [18] performed and defined a particle system as a set of autonomous individuals working together to configure the exterior of a fuzzy object like an explosion or a cloud.

In this paper, two different codes (both written in MATLAB) are linked with each other. One code is dedicated to solving the Poisson and Schrödinger equations self-consistently based on non-equilibrium Green’s function (NEGF) formalism, and the other code is dedicated to the PSO algorithm.

Although the search space is one-dimensional, it is very time-consuming to determine the optimum value of the variable by sweeping it. Sweeping of the variable usually does not lead to a precise result such as that obtained by PSO up to three decimal places.

Max iteration number for PSO in our paper is 300. Investigating the algorithm shows that after a few iterations the results for the optimum oxide thickness are repeated and the algorithm converges.

We knew the stochastic nature of the PSO algorithm used and experienced what you commented about converging to different solutions in our other works. However, in this paper, the results of the PSO algorithm were repeatable. The value of the oxide thickness very quickly converged to the best case, and this result was repeatable.

3 Simulation methodology

The Schrödinger–Poisson equations are solved self-consistently [7]. To convert the Schrödinger–Poisson equations into matrices, a finite difference scheme is used. The charge density and the density of states are calculated based on NEGF. Our proposed model can calculate the fringing fields, the potential barriers and the band-to-band tunneling. For solving the Poisson equation, the Newton–Raphson method is used.

The electrostatic potential $V(r,z)$ is obtained by solving the two-dimensional cylindrical Poisson equation [18, 19]:

$$\frac{\partial^2 V}{\partial r^2} + \frac{1}{r} \frac{\partial V}{\partial r} + \frac{\partial^2 V}{\partial z^2} = -\frac{q}{\epsilon} \rho(r,z),$$  \hspace{1cm} (1)

where $\rho(r,z)$ defines the net charge density distribution and $r$ is the CNT diameter. The net charge distribution $\rho(r, z)$ is calculated as [20]:

$$\rho\big(r = r_{CNT}, z_j\big) = \rho(z_j) - n(z_j) + N_D^- - N_A$$  \hspace{1cm} (2)

$$\rho(r \neq r_{CNT}, z) = 0,$$  \hspace{1cm} (3)

where $r_{CNT}$ is the CNT radius and $N_A^-$ and $N_D^+$ are the ionized acceptor and donor concentrations, respectively. Inside the CNT, the Poisson equation reduces to the Laplace equation, and because of the existence of charges at the CNT...
surface, the gate insulator (oxide) regions are excluded for the CNT/oxide interface. Because the potential density and charge are invariant around the nanotube, the Poisson equation is a 2D problem along the tube length ($z$) and around the radial direction ($r$).

Along the surface of the nanotube, a matching condition applied in $e$ is shown below [6, 19]:

$$
\epsilon_{\text{ins}} \frac{\partial V}{\partial r} \bigg|_{R^+} - \epsilon_0 \frac{\partial V}{\partial r} \bigg|_{R^-} = -\frac{q(p - n)}{2\pi R \epsilon_0},
$$

(4)

where the gate radius is $R^+$, the nanotube radius is $R^-$ and the insulator thickness is $t_{\text{ins}} = R^+ - R^-$. 

At the drain side of the CNTFET, Neumann boundary conditions are applied. At the normal component, the electric field at the channel–drain junction is zero. This boundary condition satisfies the charge neutrality at the source and drain junctions. The same zero electric field conditions are assumed for other boundaries. The Green function of the CNT is calculated from Eq. 5 [6, 21]:

$$
G(E) = [(E + 0^+)I - H - \Sigma_1 - \Sigma_2]^{-1},
$$

(5)

where self-energies are defined with $\Sigma_{1,2}$, $E$ is energy and $H$ is the Hamiltonian matrix.

The steps for solving the 2D Poisson equations and coupled NEGF must be repeated until a self-consistent potential is acquired. Using the Landauer–Büttiker formula, the drain current for coherent transport under a bias voltage $V$ can be calculated once self-consistency is achieved [21–23]:

$$
I = \frac{2q}{h} \int_{-\infty}^{+\infty} T(E) \left[ f(E - E_{FS}) - f(E - E_{FD}) \right] dE,
$$

(6)

where the drain-to-source transmission is defined as $T(E)$, the electron charge is $q$ and $f(E - E_{FS,FD})$ are the Fermi distribution functions at the drain and source sides.

The experimental results show in integration intervals from the limited lower value than valence band to a limited higher value above the conduction band provides accurate results. The change in this value is about 0.2–0.4 eV [6].

In order to validate the accuracy of our simulation results, we simulated the $I$-$V$ characteristic of a cylindrical transistor geometry with a wrap-around gate and a zigzag CNT with 50 nm channel length, symmetric $N$-type source and drain doping, and 8 nm thick HfO$_2$ high-$k$ gate insulator as shown in Fig. 1. To enable a fair comparison, the simulation parameters are chosen based on Javey et al. [22]. As can be seen, our results are in excellent agreement with the experimental results presented in Javey et al. [22].

### 3.1 Optimized oxide thickness for different chiralities

Figure 2 shows four cases of CNTFETs using CNTs with different chiralities. The gate oxide thickness is varied from 1 to 6 nm in steps of 1 nm, and the thickness that provides the maximum on/off current ratio is obtained.

In Fig. 2, the oxide thickness is changed manually as a discrete parametric variable.

In CNTFETs, two main mechanisms are involved in the flow of the electrons from the source to the drain: thermionic emission (TE) and tunneling. Electron transfer can occur over the top of the potential barrier between the source and the channel via the thermionic emission (TE) mechanism, or directly from the source through the channel via tunneling.

It should be noted that the general trend for the variations in the current ratio versus the oxide thickness is the same for all chiralities. That is, by increasing the oxide thickness, the current ratio increases, reaches its maximum value, and then decreases. This trend is mainly due to the variations in the off current. For small oxide thicknesses, the potential barrier height in the channel is high, so the main component of the leakage current is the tunneling mechanism. However, with an increase in oxide thickness, the TE leakage current increases while the tunneling states gradually disappear. This is because of the reduction of the gate field impact on the channel due to the energy band deformation. A further increase in oxide thickness causes the TE transport to become more probable, so the leakage current related to the TE mechanism increases and the $I_{\text{on}}/I_{\text{off}}$ ratio degrades.

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**Fig. 1** a Conventional CNTFET and b comparison between the experimental results in [22] and our simulation results.
for thicker oxides. At intermediate thickness, because of the intense reduction in the tunneling states, an increase in the current ratio occurs, where the leakage current due to tunneling decreases, and the TE leakage current is not yet dominant. This corresponds to the emergence of a peak value in the on/off current ratio plotted with respect to the oxide thickness. Therefore, by increasing the oxide thickness, first the leakage current decreases, and the $I_{\text{on}}/I_{\text{off}}$ increases. For greater thicknesses, the TE leakage can suppress the effect of the reduction in tunneling leakage, and thus no further decrease in the off-state current is observed. Therefore, the $I_{\text{on}}/I_{\text{off}}$ degradation occurs at higher oxide thicknesses.

In this paper, we aim to find the best oxide thickness that provides the maximum on/off ratio. This can be done using the PSO algorithm. Figure 3 presents the results of the PSO, which show the optimum gate oxide thicknesses for each chirality.

It is clear from the results that the lower chiral vector has a higher current ratio. In order to understand the total characteristics of the CNTFET, we have calculated other important transistor parameters including cutoff frequency and transconductance.

Table 1 shows details of the transistor behavior. It can be seen that the (7,0) chiral vector has the highest current ratio, but its cutoff frequency and transconductance are lower than that of the other chiral vectors.

Transconductance is a measure of transistor sensitivity and shows how sensitive the device current is with respect to the input voltage.
to the device voltage. It directly affects the gain of the amplifiers and their frequency responses.

The cutoff frequency shows the highest frequency at which the transistor is still working correctly. The transistor performance degrades at frequencies larger than its cutoff frequency.

Also, it is clear from the results that the (13,0) chiral vector provides a higher cutoff frequency and transconductance than other chiral vectors. The (17, 0) CNT has a much lower on/off ratio than the others. Thus, by balancing the trade-off, it seems that the (13,0) chirality provides a high cutoff frequency, large enough on/off ratio and good transconductance. Therefore, the (13,0) CNT is used for further optimization.

3.2 Optimized oxide thickness for different insulator materials

With the shrinking of transistor size due to the technical requirements for thinner gate oxides which still block the leakage current, insulator materials such as ZrO$_2$, Al$_2$O$_3$ and HfO$_2$ with higher dielectric constants have attracted attention. The use of materials with high dielectric constants will increase the mobility of electrons and holes in the channel and increase both the threshold voltage and the current of the transistors.

The simulation results for the current ratio versus the oxide thickness for different insulators are shown in Fig. 4.

We used the PSO algorithm to find the precise value for the oxide thickness for CNTFETs with different insulators, with the goal of achieving maximum current ratio. The results of the optimization are shown in Fig. 5.

As expected, the results in Fig. 5 show that the insulator with a higher dielectric constant has a higher current ratio. The optimum oxide thicknesses and their corresponding on/off ratios are also shown in Fig. 5 for each insulator. In order to better understand the behavior of the CNTFETs, other performance parameters of the optimum designs were calculated and are presented in Table. 2.

From the data in Table 2, it can be seen that the ZrO$_2$ insulator has the highest current ratio, cutoff frequency and transconductance at its optimum thickness value. Thus, it

![Fig. 4](image-url) **Fig. 4** Current ratio of the CNTFET versus oxide thickness for different types of oxide for channel length = 20 nm, (13,0) chiral vector, and $N_{sd} = 15E+08$

![Fig. 5](image-url) **Fig. 5** Variation in the current ratio of the CNTFET for different types of oxides optimized using the PSO algorithm for channel length = 20 nm, (13,0) chiral vector, and $N_{sd} = 15E+08$
can be concluded that the ZrO$_2$ insulator with a thickness of 2.722 nm is the best case among the studied designs.

### 3.3 Optimized oxide thickness for different gate lengths

The simulation results for the calculation of the current ratio versus oxide thickness for different channel lengths are shown in Fig. 6.

As can be seen in Fig. 6, shorter channel length leads to a lower current ratio. This is because of the increase in the off current. In order to calculate the precise optimum oxide thickness for each channel length, the PSO algorithm was used, and its optimization results are shown in Fig. 7.

Other important parameters are calculated and presented in Table 3. It can be seen that a channel length of 30 nm obtains a higher current ratio than other structures at optimum oxide thickness. However, at this optimum oxide thickness, the 30 nm channel length has a slightly lower cutoff frequency than lengths of 10 nm and 20 nm, while the transconductance is similar to that for other channel lengths.

#### Table 2  PSO algorithm results of different parameters at optimized oxide thickness

| Parameter/type | ZrSiO$_4$ (5) | HfSiO$_4$ (11) | HfO$_2$ (16) | ZrO$_2$ (25) |
|----------------|---------------|----------------|--------------|--------------|
| $t_{\text{ins}}$ (nm) | 1.498 | 1.773 | 2.043 | 2.722 |
| Ion/Ioff | 2.97E+05 | 8.08E+05 | 1.16E+06 | 1.95E+06 |
| Cutoff frequency | 1.55E+12 | 1.94E+12 | 2.11E+12 | 2.31E+12 |
| Transconductance | 3.21E−04 | 5.48E−04 | 6.79E−04 | 8.41E−04 |

Fig. 7 The optimized current ratio variation of the CNTFET for different channel lengths using the PSO algorithm for (13,0) chiral vector, $\epsilon_{\text{ins}} = 16$, and $N_{sd} = 15E+08$

### 3.4 Optimized oxide thickness for different doping concentrations

In this section, the oxide thickness is optimized for different doping concentrations. The simulation results for the current ratio versus oxide thickness for different doping concentrations are shown in Fig. 8.

In Fig. 8, for each doping concentration, the oxide thickness is varied and the on/off ratio is calculated. However, in order to determine the exact optimum oxide thickness which corresponds to the maximum on/off ratio, the PSO algorithm is used. The outputs of the PSO are shown in Fig. 9.
It is clear from Fig. 9 that the highest current ratio is obtained for $N_{sd} = 1E+08$ source and drain doping concentration. Other important parameters for CNTFET with $N_{sd} = 1E+08$ are also calculated and are shown in Table 4.

The simulation results show that the optimum doping level with the optimized insulator thickness improves the device performance. It can be seen in Table 4 that the source and drain doping concentration $N_{sd} = 1E+08$ provides a higher current ratio, cutoff frequency and transconductance than other doping levels at the optimum oxide thickness. The optimized high-performance CNTFETs designed based on the obtained results are proposed in next section.

### Table 3 PSO algorithm results for different parameters at optimized oxide thickness

| Parameter/type | $L_g = 10$ nm | $L_g = 20$ nm | $L_g = 30$ nm | $L_g = 40$ nm |
|----------------|----------------|----------------|----------------|----------------|
| $t_{ins}$ (nm) | 1.903          | 2.043          | 2.581          | 2.581          |
| $I_{on}/I_{off}$ | 1.50E+04      | 1.16E+06      | 1.69E+06      | 1.22E+06      |
| Cutoff frequency | 3.53E+12       | 2.11E+12       | 1.60E+12       | 1.27E+12       |
| Transconductance | 6.9E−04       | 6.79E−04       | 6.75E−04       | 6.75E−04       |

### Fig. 8 Current ratio of the CNTFET versus different oxide thicknesses for different doping levels for a (13,0) chiral vector, $\text{eps}_{ins} = 16$, and channel length = 20 nm

### Fig. 9 The optimized current ratio of the conventional CNTFET for different doping concentrations using the PSO algorithm at $V_D=0.5$ V

### 4 Proposed optimized CNTFETs

In this section, based on the optimum values and the results obtained in previous sections, two CNTFET structures with different chiral vectors are proposed.

The design parameters and the DC and AC characteristics of the proposed CNTFET with a (7,0) chiral vector are shown in Table 5. As can be seen, for a CNT with length...
of 30 nm, oxide thickness of 3.114 nm and dielectric constant of 25, the on/off ratio reaches 5.73E+09, and a cutoff frequency of 4.03E+11 Hz is obtained. To further understand the behavior of the device, additional parameters of power–delay product (PDP) and delay are also shown in Table 5.

The same procedure is used to obtain high performance using a (13,0) CNTFET. The design parameters of the proposed CNTFET are shown in Table 6.

It is notable from the comparison between Tables 5 and 6 that the (7,0) chiral vector has a larger current ratio and delay and lower cutoff frequency and transconductance. This is due to the different bandgap of the CNTs used in these structures.

The results show that oxide thickness should be selected very carefully in CNTFET design, and not based only on previously reported values in other works. Each design requires its own optimum oxide thickness that provides the maximum on/off current ratio, which is one of the electrical figures of merit (FOM) for the optimized structure. The current ratio is an important FOM for digital device applications, while transconductance \((g_m)\) plays an important role in analog applications where amplification is necessary. Therefore, it is not necessary or even practical to optimize a device for both applications.

5 Conclusion

This work has shown that most studies investigating CNTFETs have neglected the importance of the optimum value of oxide thickness. In this paper, the optimum oxide thicknesses were calculated based on the PSO algorithm with the objective of maximizing the on/off current ratio of the CNTFETs. The results showed that due to changes in the contributions of the tunneling and thermionic emission leakage currents with changes in the oxide thickness, each CNTFET has a peak on/off ratio with an intermediate oxide thickness. Most importantly, by changing the chirality, channel length, doping concentration and insulator type, the optimum value

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**Table 4** PSO algorithm for different parameters at optimized oxide thickness

| Parameter/type    | \(N_{sd} = 3E+07\) | \(N_{sd} = 1E+08\) | \(N_{sd} = 1.5E+09\) | \(N_{sd} = 3E+09\) |
|------------------|-------------------|-------------------|-------------------|-------------------|
| \(t_{ins}\) (nm) | 3.098             | 2.154             | 2.043             | 12.7753           |
| \(I_{on}/I_{off}\) | 1.08E+07          | 5.43E+07          | 1.16E+06          | 2.92E+04          |
| Cutoff frequency | 2.73E+12          | 3.45E+12          | 2.11E+12          | 2.41E+12          |
| Transconductance | 8.32E–05          | 8.25E–04          | 6.79E–04          | 2.60E–03          |

**Table 5** PSO algorithm for the first proposed structure with optimized oxide thickness and a \((7,0)\) chiral vector

| Parameter/type | \(I_{on}/I_{off}\) | Cutoff frequency | Transconductance | PDP     | Delay       |
|----------------|-------------------|-----------------|----------------|--------|-------------|
| \(N_{sd} = 1E+08\) | 5.73E+09          | 4.03E+11        | 4.59E–08       | 4.94E+20 | 3.96E+10    |
| \(L_g = 30\) nm     |                   |                 |                |        |             |
| \(\varepsilon_{ins} = 25\) |               |                 |                |        |             |
| Chiral vector = \((7,0)\) |             |                 |                |        |             |
| \(t_{ins} = 3.114\) nm |               |                 |                |        |             |

**Table 6** PSO algorithm for the second proposed structure with optimized oxide thickness and a \((13,0)\) chiral vector

| Parameter/type | \(I_{on}/I_{off}\) | Cutoff frequency | Transconductance | PDP     | Delay       |
|----------------|-------------------|-----------------|----------------|--------|-------------|
| \(N_{sd} = 1E+08\) | 7.21E+07          | 2.03E+12        | 1.50E–03       | 6.33E–19 | 1.69E–13    |
| \(L_g = 30\) nm     |                   |                 |                |        |             |
| \(\varepsilon_{ins} = 25\) |               |                 |                |        |             |
| Chiral vector = \((13,0)\) |             |                 |                |        |             |
| \(t_{ins} = 11.4\) nm |               |                 |                |        |             |

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for the oxide thickness changes. By calculating the transconductance and cutoff frequency as well as the on/off ratio, the whole device performance was investigated. It was shown that CNTFET characteristics are highly dependent on the oxide thickness, which significantly affects the AC and DC performance.

Authors’ contributions 1: Study concept and design; data acquisition; statistical analysis; Analysis and interpretation of data. 2: Study supervision; Administrative, technical, and material support; Critical revision of the manuscript for important intellectual content. 3: Revision of the manuscript for important intellectual content. All authors read and approved the final manuscript.

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Declarations

Conflict of interest All authors listed in this paper certify that they have no affiliation with or involvement in any organization or entity with any financial interest or nonfinancial interest in the subject matter or any materials discussed in this manuscript.

Ethical approval This article does not contain any studies with human participants or animals performed by any of the authors.

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