

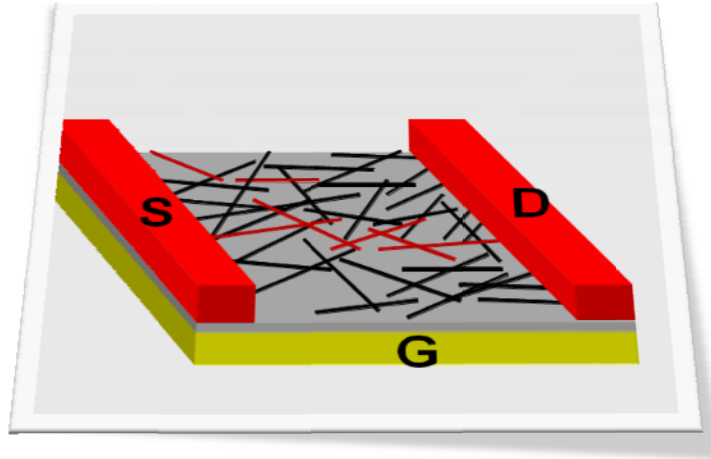
NanoNet : A Computational Tool for Electro-Thermal Transport in Carbon Nanotube Network Transistors

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1. INTRODUCTION

NanoNet tool simulates electrical and thermal transport in a Carbon nanotube network thin film transistors (CN-TFTs). The CN-TFTs have been investigated for potential applications in large-area macro-electronics on plastic or glass such as liquid crystal displays, e-paper, chem-bio sensors, solar cells and shape-conformable antennae and radar¹⁻¹². The channel of these thin-film transistors consists of random network of thousands of nanotubes percolating from the source to drain electrodes^{4, 5, 13, 14}. However, partially aligned or fully aligned CNT arrays have also been investigated and offer an attractive solution for applications that require very high performance^{11, 12, 15, 16}. The NanoNet tool calculates the current through this interpenetrating network of random or partially aligned carbon nanotubes by solving drift-diffusion and the Poisson equations^{6, 7, 17}. The tool provides the capability to analyze the effect of key device parameters such as channel length, channel width, tube length, network density, and conductive parameters such as tube-to-tube coupling strength. In some application such as transparent displays, CN-TFTs can be covered by the insulating materials (~ glass, polymer, etc.). Self-heating may become a concern for such applications especially if the requirements of flexibility forbid the use of active cooling⁶. The nanoNet tool provides an option of exploring peak temperature as well as the temperature distribution in a NB-TFT as a function of important device parameters such as tube density and/or channel length.

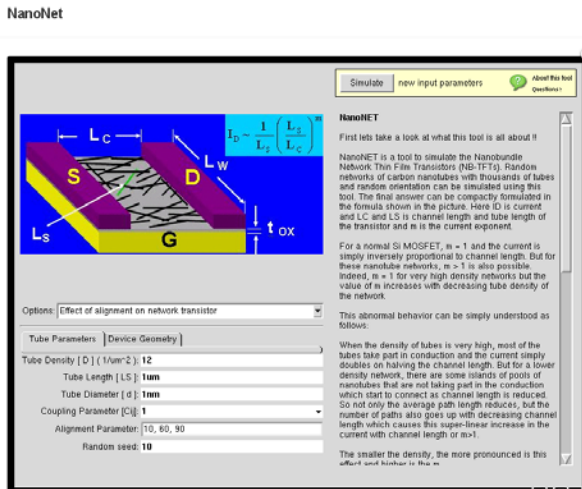


Figure 1. A snapshot of nanoNet tool.

2. BASICS OF NANONET THIN FILM TRANSISTOR

2.1 Device Geometry

The geometrical parameters of a NB-TFT are defined in Figure 2. L_C is the channel length between source and drain contacts, L_W is the channel width, L_S is the tube length, t_{ox} is the dielectric thickness between gate and channel of the device. These parameters can be provided as inputs to the nanoNet tool. The dependence of drain current on L_C and L_S can be summarized by an analytical formula shown in the upper right corner of Figure 2 (m is the current exponent)^{17, 18}. The numerical results from the Nanonet simulation should be compared against such analytical results to ensure the correctness of the solution.

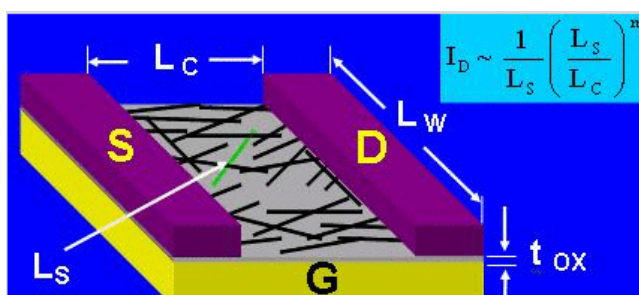


Figure 2. A schematic of NB-TFT with source, drain, gate and channel regions. Percolating network of CNTs connect source and drain contacts. L_C is the channel length, L_W is the channel width, and L_S is the tube length (see green line).

2.2 Orientation of CNT network

CNT network can be oriented or arranged in different ways inside a channel region of TFT. The orientation of CNT network can be characterized by an alignment parameter Θ , which is defined as the average of the angle nanotube axes make with a horizontal line connecting source to drain. $\Theta=0$ corresponds to a completely aligned network and $\Theta=90$ corresponds to a random network (see Figure 3).

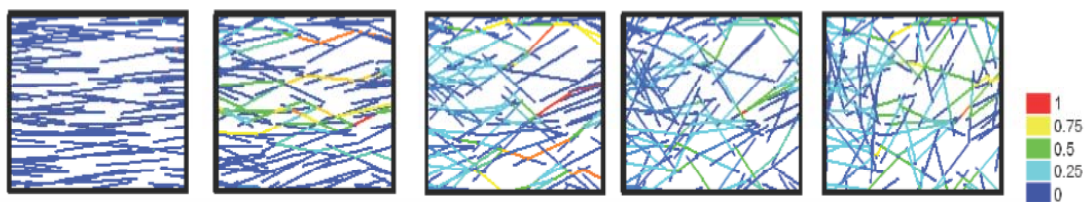


Figure 3. CNT networks of different orientations. The first figure from left is aligned network ($\Theta=0$); the last figure is random network ($\Theta=90$); other figures in middle corresponds to $0 < \Theta < 90$.

2.3 Governing Equations

Electrical Transport: The current through a NB-TFT device of a specified geometry is determined by solving the drift-diffusion equations and the Poisson equation^{6, 7}. In the ‘bottom-up’ description of the channel, the drift-diffusion and Poisson equations are generalized for CN-TFTs as:

$$\left. \begin{aligned} \frac{d^2\Phi}{ds^2} + \frac{\rho}{\varepsilon} &= 0 \\ \nabla \cdot \mathbf{J}_p &= 0 \\ \nabla \cdot \mathbf{J}_n &= 0 \end{aligned} \right\} \rightarrow \begin{aligned} \sum_{i=1}^N \left(\frac{d^2\Phi_i}{ds^2} + \frac{\rho_i}{\varepsilon} - \frac{(\Phi_i - V_G)}{\lambda^2} + \sum_{j \neq i} \frac{(\Phi_j - \Phi_i)}{\lambda_{ij}^2} \right) &= 0, \\ \sum_i \left(\nabla \cdot \mathbf{J}_{pi} + \sum_{j \neq i} C_{ij}^p (p_j - p_i) \right) &= 0, \\ \sum_i \left(\nabla \cdot \mathbf{J}_{ni} + \sum_{j \neq i} C_{ij}^n (n_j - n_i) \right) &= 0, \end{aligned} \quad (1)$$

where, N is total number of CNTs, s is in the direction of individual CNT, ρ is total charge density, and the term $-(\Phi - V_G) / \lambda^2$ (the well known parabolic approximation) introduces the effect of the back gate, where λ is effective screening length. The term $(\Phi_j - \Phi_i) / \lambda_{ij}^2$ is the tube-tube interaction with screening length λ_{ij} where a node on tube i intersects a node on tube j . The additional term $C_{ij}^n (n_j - n_i)$ in the continuity equation representing charge transfer between nanotubes at the point of intersection^{7, 19}.

Thermal Transport: The NB-TFT device is assumed to be embedded inside a low thermal conductivity matrix (or substrate) and heat generated in the device is removed from the top and bottom surfaces of this matrix by natural convection. This geometry represents a typical pixel of the electronic display⁶. A diffusive modeling framework is used to simulate the thermal transport in the network of CNT transistor and the pixel matrix in which the CNT transistor is embedded. Fourier conduction equations²⁰ are solved for estimating the temperature distribution in the system. Conduction equations for a 3D system can be written as:

$$\nabla(k\nabla T) + q''' = 0 \quad (2)$$

Using the dimensionless variable, $\theta = (T - T_{inf}) / (Q' d L_t / k_t)$, for the temperature and non-dimensionalizing all lengths by the tube diameter d , the governing conduction equations in the tubes and substrate may be written as⁶:

$$\frac{d^2\theta_i}{ds^{*2}} + \sum_{\text{intersecting tubes } j} Bi_c (\theta_j - \theta_i) + Bi_s (\theta_s - \theta_i) + \frac{d}{L_S} \frac{q_i'}{Q} = 0 \quad (3)$$

$$\nabla^{*2}\theta_s + \sum_{i=1}^{N_{tubes}} Bi_s \beta_v (\theta_i - \theta_s) = 0 \quad (4)$$

Here, T_{inf} is the ambient temperature, q'_i is the Joule heating term inside the nanotube with units of power per unit volume and Q' is the reference power per unit volume which is used for non-dimensionalizing the temperature term in the heat transport equation. L_S is the length of the tube and k_t is the thermal conductivity of the tube. $\theta_i(s^*)$ is the non-dimensional temperature of the i_{th} tube at the axial location s^* , and $\theta_s(x^*, y^*, z^*)$ is the substrate temperature. Thermal contact between tubes i and j is characterized by the contact Biot number Bi_C . Heat exchange between each tube and the substrate is governed by the substrate Biot number Bi_S and the contact parameter β . The second term in Eq. (3) for CNT temperature represents tube-tube interaction and the third term represents tube-substrate interaction. The second term in Eq. (4) for substrate temperature represents tube-substrate interaction.

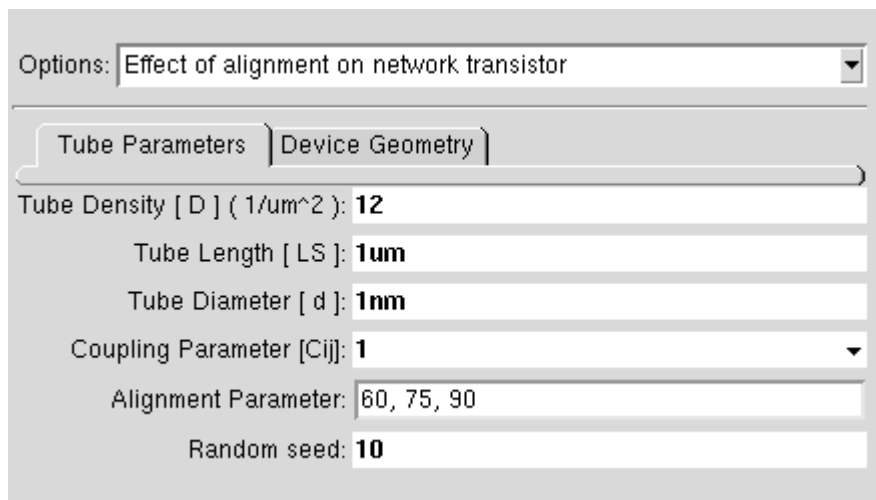
3. DESCRIPTION OF TOOL

NanoNet tool provide multiple options to analyze the CN-TFTs as function of different geometrical and conductions parameters. Three options available in the current nanoNet tool are (i) Effect of alignment on network transistor, (ii) Current Scaling with channel length, and (iii) Temperature distribution in CNT network. The details of these options and entries required in subpanels are described below.

‘*Tube Parameters*’ subpanel for all three options allows to input numerical values of different parameters for the CNT-network such as tube density, tube diameter, coupling parameter, alignment parameter and random seed (Figure 4, top). Alignment parameter (Θ) is described in section 2.2. Coupling parameter can be selected between 0 and 1. Here, 1 corresponds to very good contact between nanotubes and 0 corresponds to no coupling. A very small value ($\sim 10^{-7}$) should be provided as input to represent weak coupling rather than inputting 0.

‘*Device Geometry*’ subpanel allows inputting numerical values of different parameters for the device geometry such as channel length, channel width, gate oxide thickness and dielectric constant (Figure 4, bottom).

Note: If the input for tube density is less than the percolation threshold density, then CNT network may not connect from source to drain leading to zero current or divergence in numerical simulations. It is suggested that *tube densities higher than $10 \mu\text{m}^2$* and *channel length lower than $10 \mu\text{m}$* be given as inputs in subpanels to avoid such divergence. Users should use lecture notes at nanoHUB²¹ to estimate the percolation threshold density. Instead of giving a long simulation with many parameters, we suggest that the user do one thing at a time, understand the results, and then do the next simulation.



Options: Effect of alignment on network transistor

Tube Parameters | Device Geometry

Tube Density [D] (1/um²): 12

Tube Length [LS]: 1um

Tube Diameter [d]: 1nm

Coupling Parameter [Cij]: 1

Alignment Parameter: 60, 75, 90

Random seed: 10

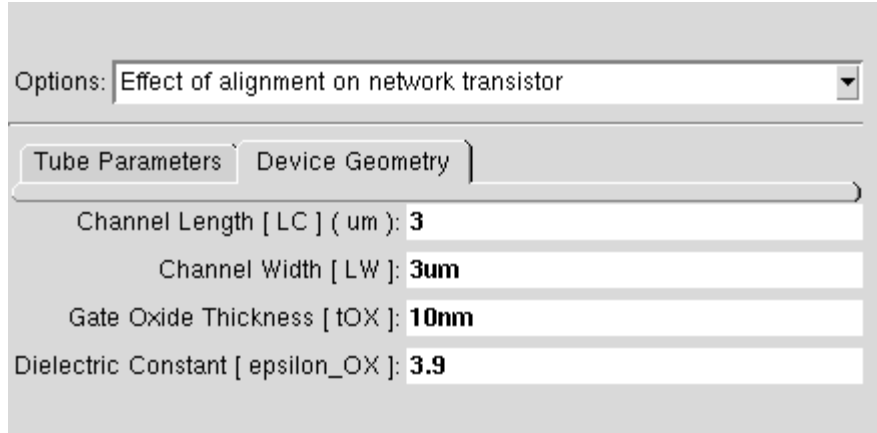


Figure 4. GUI for option ‘Effect of alignment on network transistor’. Top figure is for ‘Tube Parameters’ and bottom figure for ‘Device Geometry’.

3.1 Effect of alignment on network transistor

This option in nanoNet tool allows analyzing the effect of tube orientation on current through the device. The tube orientation can be changed by changing alignment parameter in ‘Tube Parameters’ subpanel in the range of 0-90 (see Figure 4, top). As an output, the current distribution through the network in non-dimensional units can be visualized; plot of ‘current ~ alignment parameter’ will be also available once simulations get completed.

3.2 Current Scaling with channel length

This option allows analyzing the effect of increasing channel length (L_C) on current through the device for different tube densities. Multiple values of channel length (L_C) and tube densities can be provided as inputs in subpanels (see Figure 5). This option has an additional subpanel ‘Statistics’ where number of samples (\sim) can be provided as inputs. The tool provides output results by averaging the results of all successful simulations. Simulations may fail for some samples if tube density $<$ percolation threshold densities; results of these samples are discarded. Plot of ‘current ~ L_C ’ will be available once all simulations get completed. Current exponents (m) can be also observed in the legend of these plots (see section 2.1).

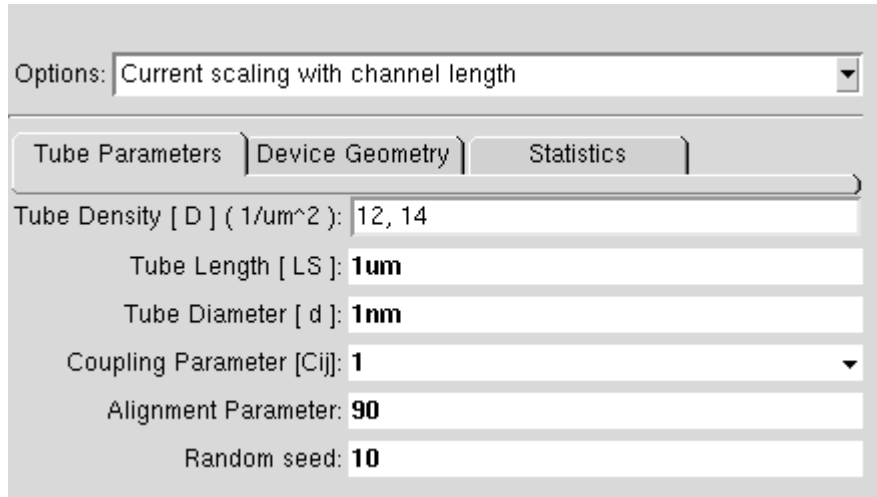


Figure 5. GUI for option ‘Current scaling with channel length’

3.3 Temperature distribution in CNT network

This option in nanoNet tool allows analyzing the temperature distribution in CNT-network and peak temperature of the device. Multiple values of channel length (L_C) and tube densities can be provided as inputs in subpanels (see Figure 6). This option also has an additional subpanel ‘Statistics’, where number of samples (\sim) can be provided as input. As an output, the temperature distribution through the network can be visualized; plots of ‘current $\sim L_C$ ’ and ‘peak temperature $\sim L_C$ ’ will be also available once simulations are completed.

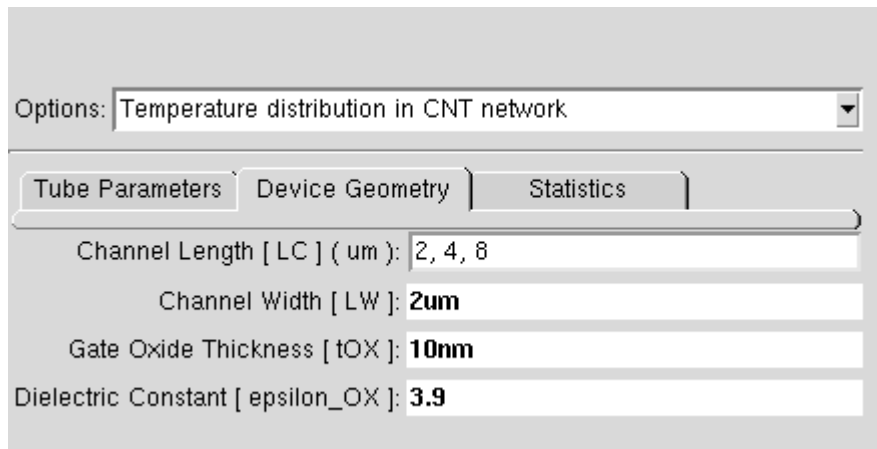


Figure 6. GUI for option ‘Temperature distribution in CNT network’

4. EXAMPLE PROBLEMS

4.1 Effect of alignment

Example 1: Estimate current distribution in a NB-TFT for $L_C = 5 \mu\text{m}$, $L_S = 1 \mu\text{m}$, and alignment parameter (Θ) in the range of 0-45.

Answer:

GUI Input

Step 1: In the options menu, select ‘Effect of alignment on network transistor’ from the three options available and then click on tab ‘Tube Parameters’. The GUI will look similar to as shown below. Tube density, tube length, tube diameter, coupling parameter, alignment parameter and random need to be selected from this menu. The tube density should be selected greater than the percolation threshold density and different values of alignment parameter between 0-90 and a coupling parameter between 0-1 can be selected. For, this case, select tube density = $12 \mu\text{m}^2$, alignment parameter as 0, 5, 10, 15, 20, 25, 30, 35, 40 and 45 and coupling parameter as 1. Other parameters can be left to their default values.

Options: Effect of alignment on network transistor

Tube Parameters | Device Geometry

Tube Density [D] (1/um²): 12

Tube Length [LS]: 1um

Tube Diameter [d]: 1nm

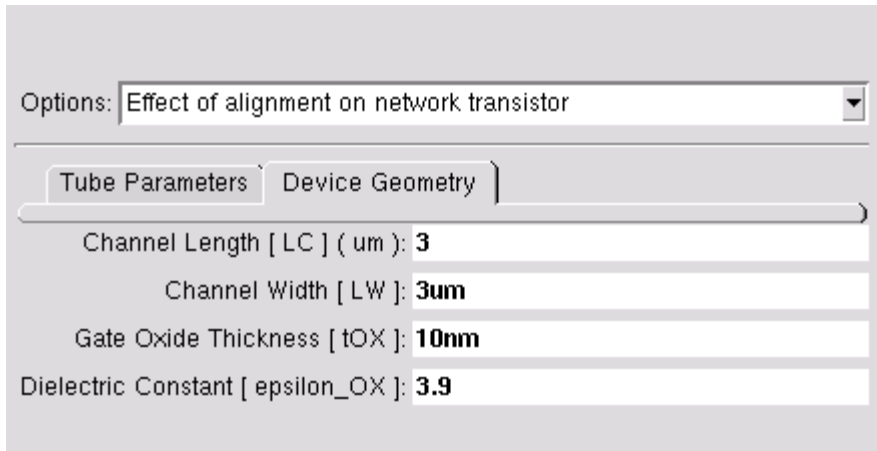
Coupling Parameter [Cij]: 1

Alignment Parameter: 60, 75, 90

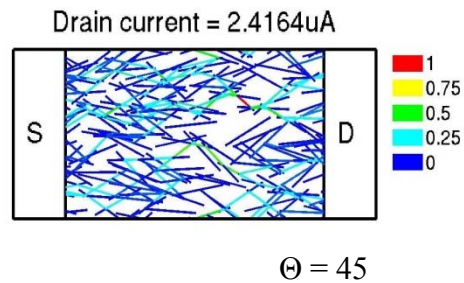
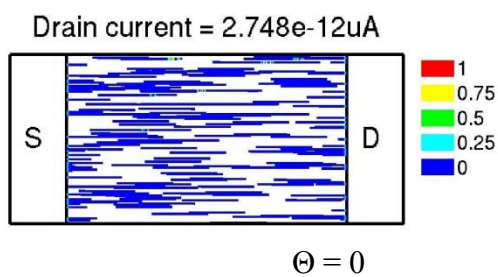
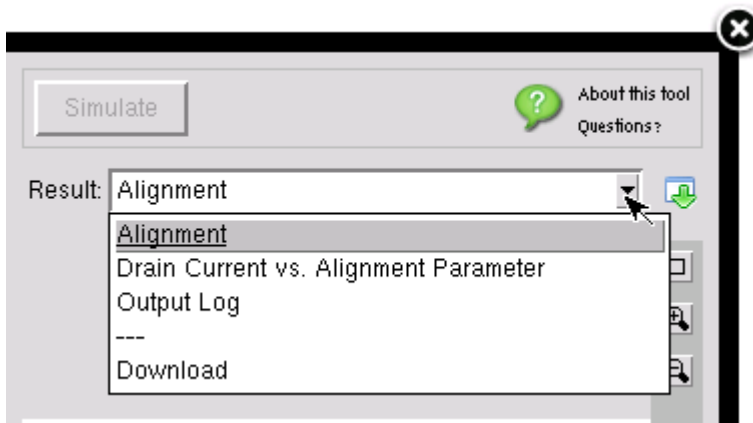
Random seed: 10

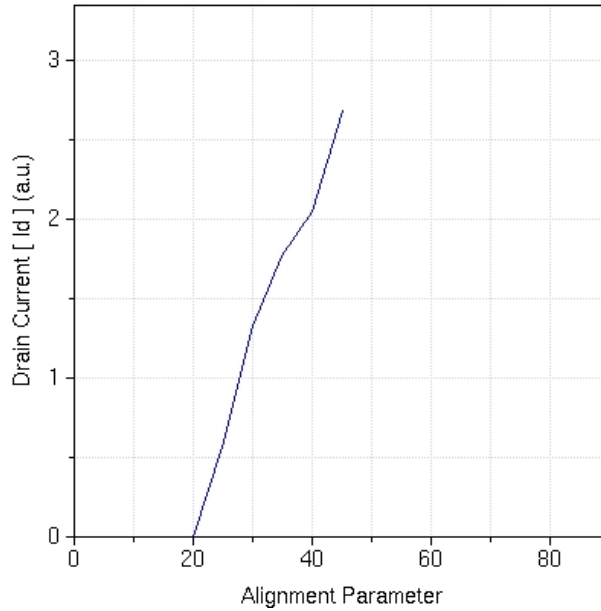
Step 2: Now move to tab ‘Device Geometry’. The GUI will look similar to as shown below. Channel length, channel width, gate oxide thickness and dielectric constant need to be selected from this menu. For, this case, select channel length = $5 \mu\text{m}$, channel length = $3 \mu\text{m}$ and other parameters can be left to their default values.

Now click on simulate tab to submit the job.



Once the simulations are over, the voltage distribution and drain current ~ alignment parameter can be analyzed from the output menu shown below.





Comments. The results show that the alignment reduces total current through the network. This counterintuitive result reflects the fact while alignment reduces average path length between source and drain, the number of such paths connected between source and drain are reduced dramatically with alignment (top, left). For further details, see Reference [18].

Simulation Time: 8 minutes using one processor for ten different orientations ($\Theta = 0-45$ at interval of 5) considered here.

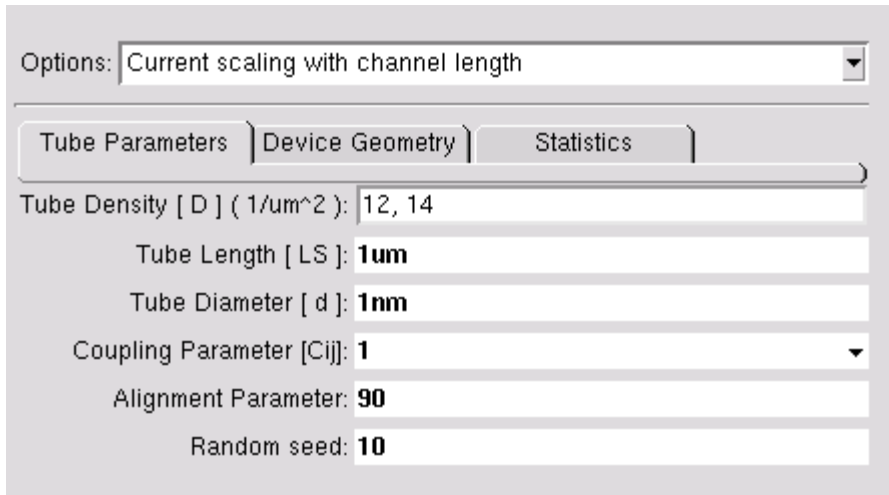
4.2 Scaling with channel length

Example 2: Estimate current flow through a NB-TFT for $L_C = 2, 4, 6,$ and $8 \mu\text{m}$, $L_S = 1 \mu\text{m}$, and for two different tube densities ($10 \mu\text{m}^2$ and $14 \mu\text{m}^2$). What are the current exponents (m) for these two different densities?

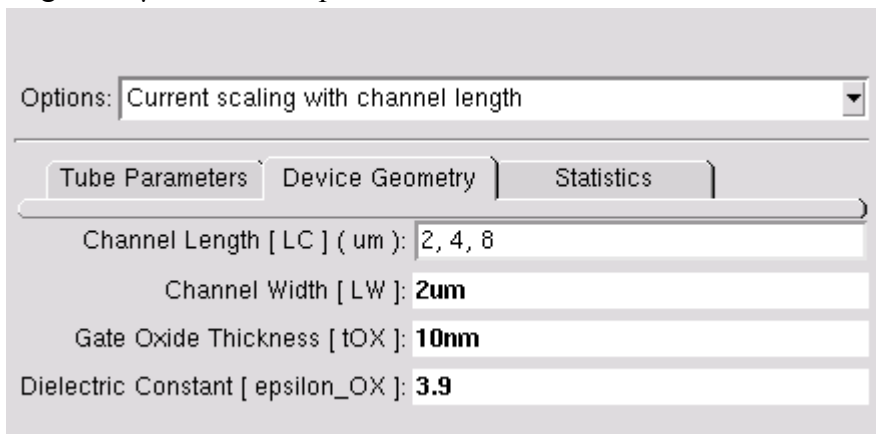
Answer:

GUI Input

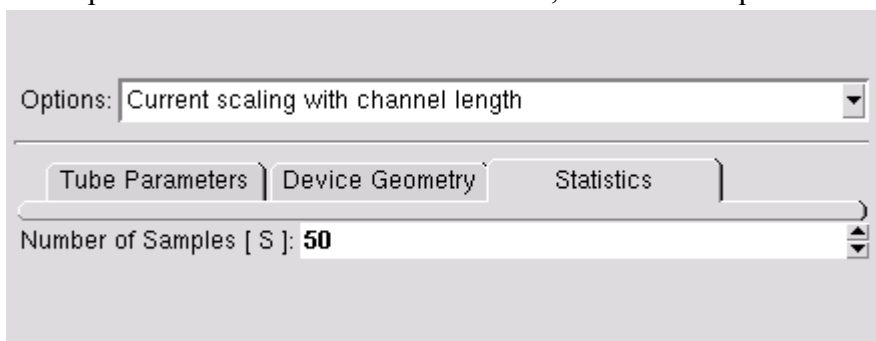
Step 1: In the options menu, select ‘Current scaling with channel length’ from the three options available and then click on tab ‘Tube Parameters’. The GUI will look similar to as shown below. Tube density, tube length, tube diameter, coupling parameter, alignment parameter and random need to be selected from this menu. For, this case, select tube density = 10, 14 (μm^2), alignment parameter as 90 (~ random orientation) and coupling parameter as 1. Other parameters can be left to their default values.



Step 2: Now move to tab ‘Device Geometry’. The GUI will look similar to as shown below. Channel length, channel width, gate oxide thickness and dielectric constant need to be selected from this menu. For, this case, select channel length = 2, 4, 6, 8 (μm), channel length = 2 μm and other parameters can be left to their default values.

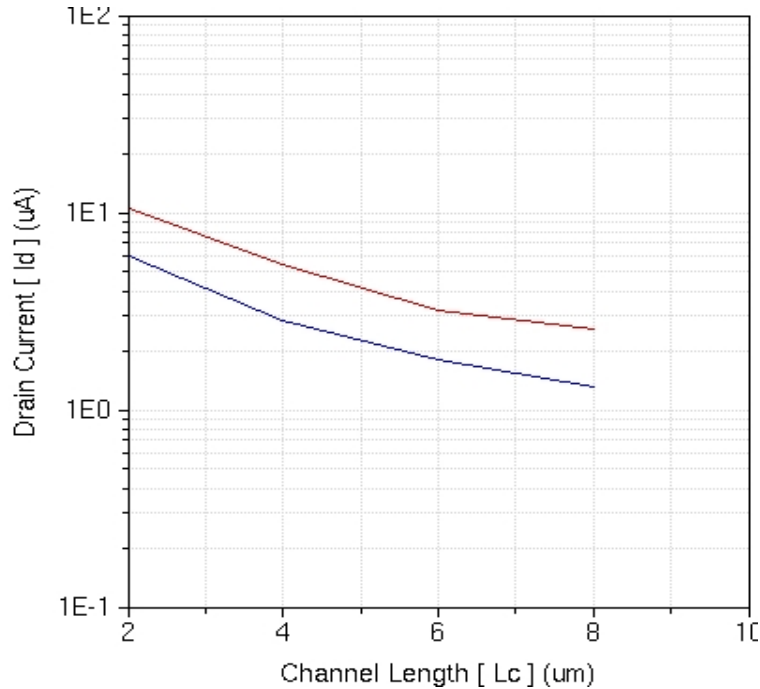


Step 3: Now move to tab ‘Statistics’. The GUI will look similar to as shown below. Number of samples need to be selected. In this case, select 25 samples.



Now click on simulate tab to submit the job.

Once the simulations are over, the drain current ~ channel length can be analyzed from the output menu.



Density = 10 μm^2 (blue curve) and Density = 14 μm^2 (red curve).

The current through the device has following dependence^{7, 18} on channel length (L_C) and tube length (L_S): $I_D \sim 1/L_S [L_S/L_C]^m$. The exponent, m , can be obtained from the slope of the curve: $\log(I_D) \sim \log(L_C)$, i.e., m can be obtained from the slope of the $I_D \sim L_C$ curve in the logarithmic units. For a normal Si MOSFET, $m = 1$ and the current is simply inversely proportional to channel length. But for nanotube networks, $m > 1$ is also possible. Indeed, $m = 1$ for very high density networks but the value of m increases with decreasing tube density of the network.

In the present example, the current exponent (m) for the curve corresponding to density= $10 \mu\text{m}^2$ is 1.103 and for density= $14 \mu\text{m}^2$ is 1.034.

Simulation Time: 5 minutes using 25 processors for two different densities ($10 \mu\text{m}^2$ and $10 \mu\text{m}^2$) and four different channel lengths (2 μm , 4 μm , 6 μm , and 8 μm) considered here.

4.3 Temperature distribution

Example 3: Estimate temperature distribution in a NB-TFT for L_C in the range of 2-10, μm , $L_S = 1 \mu\text{m}$, and for two different tube densities ($10 \mu\text{m}^2$ and $14 \mu\text{m}^2$). Plot peak temperature and current against channel length for these two different densities?

Answer:

GUI Input

Step 1: In the options menu, select ‘Temperature distribution in CNT network’ from the three options available and then click on tab ‘Tube Parameters’. Tube density, tube length, tube diameter, coupling parameter, alignment parameter and random need to be selected from this menu. For, this case, select tube density = 10, 14 (μm^2), alignment parameter as 90 (~ random orientation) and coupling parameter as 1. Other parameters can be left to their default values.

Step 2: Now move to tab ‘Device Geometry’. Channel length, channel width, gate oxide thickness and dielectric constant need to be selected from this menu. For, this case, select channel length = 2, 4, 6, 8, 10 (μm), channel length = 2 μm and other parameters can be left to their default values.

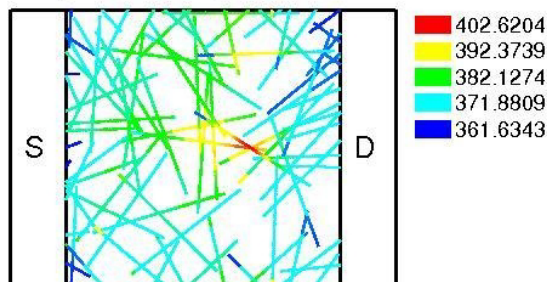
Step 3: Now move to tab ‘Statistics’. The GUI will look similar to as shown below. Number of samples need to be selected. In this case, select 25 samples.

Note: GUI for this case corresponding to different tabs are same as shown in example-2 and has not been repeated here for brevity.

Now click on simulate tab to submit the job.

Once the simulations are over, temperature contours in CNT network, drain current ~ channel length, and temperature ~ channel length can be analyzed from the output menu.

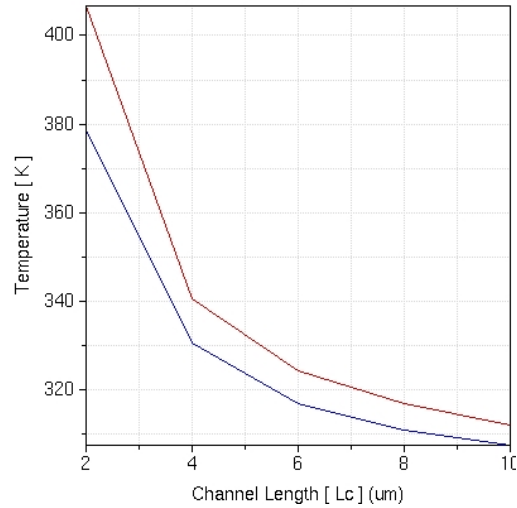
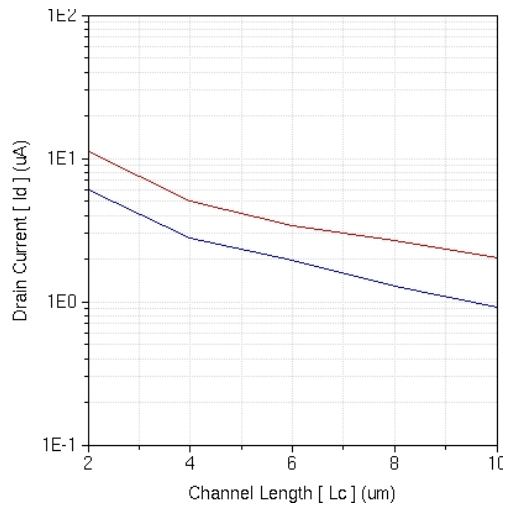
$L_C = 2\mu\text{m}$, $L_W = 2\mu\text{m}$, $D = 14 \text{ tubes}/\mu\text{m}^2$



$L_c = 6\mu\text{m}$, $L_w = 2\mu\text{m}$, $D = 14 \text{ tubes}/\mu\text{m}^2$



$L_c = 8\mu\text{m}$, $L_w = 2\mu\text{m}$, $D = 14 \text{ tubes}/\mu\text{m}^2$



Density = $10 \mu\text{m}^2$ (blue curve) and Density = $14 \mu\text{m}^2$ (red curve)

Simulation Time: 15 minutes using 25 processors for two different densities ($10 \mu\text{m}^2$ and $10 \mu\text{m}^2$) and five different channel lengths ($2 \mu\text{m}$, $4 \mu\text{m}$, $6 \mu\text{m}$, $8 \mu\text{m}$ and $10 \mu\text{m}$) considered here.

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6. FREQUENTLY ASKED QUESTIONS

Q1. What is V_G and V_D ?

A. V_G is the voltage between gate-to-source electrodes and V_D is the voltage between drain-to-source electrodes.

Q2. What is current exponent?

A. The current through the NB-TFT device can be expressed as function of channel length (L_C) and tube length (L_S): $I_D \sim 1/L_S [L_S/L_C]^m$. Here, m is defined as the current exponent (see section 4.2 for more details).

Q3. What is the reason that sometimes the simulations do not converge?

A. This may be due to the following reasons: (i) tube density is too low, (ii) very large channel length or tube density has been selected, (iii) very low charge transfer coefficient C_{ij} has been selected. See section 3, “Description of the Tools” for guidance on the selection of these parameters.

Q4. How many processors should I select for a simulation?

A. The tool estimates the number of processors needed to perform the simulations in reasonable timeframe based on the parameters provided as inputs in GUI.

Q5. How long the simulations will run?

A. The total time required for the simulations depends on the variables provided as inputs in the GUI such as tube density, channel length, number of samples, etc. Example problems in section 4 suggest approximate time required corresponding to the inputs in these examples. These examples can be used as guidelines to estimate the approximate time for the requested simulations. However, this simulation time represent the time of execution of the jobs. Jobs may be put into queue before the actual execution starts and total time may be longer than the estimated time depending on how busy are the servers during the job submission.

Q6. Can we track the status of submitted jobs ?

A. The GUI provides the current status in terms of the % of the simulations completed. In addition, it also gives information about how many jobs queued, submitted or running.

Q7. What is the alignment parameter in GUI ?

A. The alignment parameter (θ) characterizes the orientation of CNT network. This is defined as the average of the angle nanotube axes make with a horizontal line connecting source to drain (see section 2.2 for details).

Q8. What is the coupling parameter in GUI ?

A. The coupling parameter is charge transfer coefficient (C_{ij}) at CNT-CNT junctions (see section 2.3 for details).

Q9. What is the random seed in GUI ?

A. This is a parameter for the random orientation of the network. If seed is selected as 0, then tool will select a different random orientation of the network every time simulation is executed. For a non-zero random seed, the network orientation and results will be exactly same if same set of parameters are selected.

7. LIMITATIONS AND NEW FEATURES OF THE CURRENT VERSION

1. The current version of the ‘nanonet tool’ assume diffusive charge transport through the CNT network and solve for current and potential distribution using drift-diffusion and Poisson equations. This assumption may break when channel length is very small and ballistic charge transport become dominant.
2. At present, simulation tool only consider low values of drain voltage V_D (~linear regime).
3. Diffusive thermal transport in the CNT-network has been assumed as phonon boundary scattering at CNT interfaces dominate the thermal transport through the network.
4. Charge transfer coefficient (C_{ij} in Eq. (1)) at CNT-CNT junctions is assumed to be constant in the entire CNT-network.
5. The contact thermal conductance between CNTs (B_{iC} in Eq. (3)) and between CNT-substrate (B_{iS} in Eq. (3)) is assumed to be constant in the entire CNT-network.
6. The simulations may diverge if the tube density is below the percolation threshold density (~ tube network is not percolating from source-to-drain which means zero current at any voltage), if tube density or channel length is very high and the memory required for the simulations are beyond the hardware limitations or if extremely small charge transfer coefficient (C_{ij}) is selected.
7. All CNTs in a CNT-network are assumed to be straight without any crimples.

New Features

1. The current version of the nanoNet tool includes a new option: ‘Temperature Distribution in CNT Network’. This new option in the tool allows analyzing the temperature distribution in CNT-network as a function of different device parameters such as channel length and tube density. Users can visualize the temperature distribution through the network and can save plots of ‘current ~ L_C ’ and ‘peak temperature ~ L_C ’ for the inputs provided in GUI once simulations are completed using this option.