Statistic Analysis of Nanoscale Tunneling Electrical Contacts Based on Transmission Line Model

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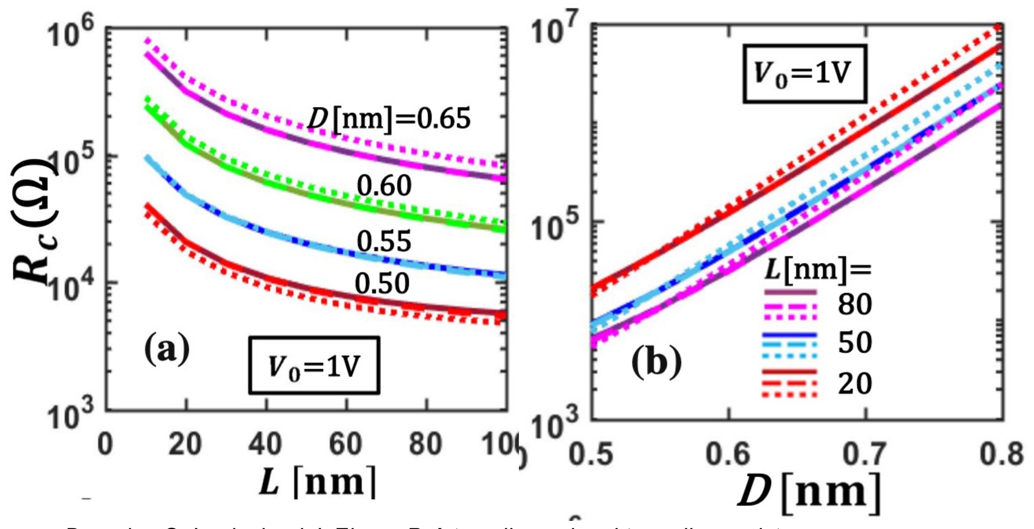
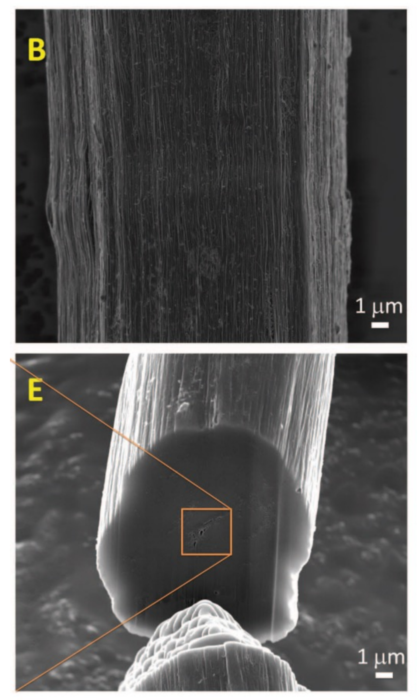
I. Motivation

- Contact engineering is very significant in innovative electronic circuits that utilize graphene, carbon nanotubes (CNTs), and other emergent materials. Specifically, devices built on CNTs face pronounced obstacles stemming from the connections between the tubes.
- By coupling the transmission line model and tunneling current, a self-consistent contact model was established to solve the current and voltage distribution along the contact length and the overall contact resistance for various electrical contact dimensions (contact length and thickness of interface layer).



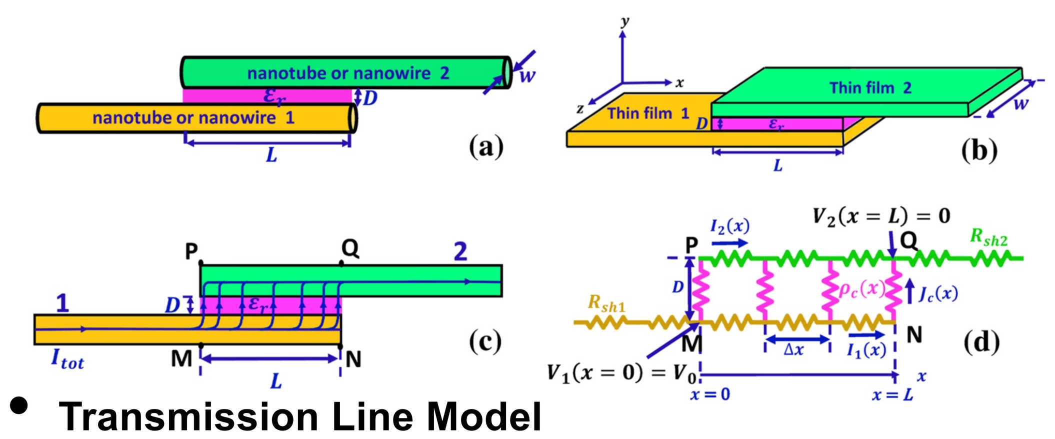
Banerjee S, Luginsland J, Zhang P. A two dimensional tunneling resistance transmission line model for nanoscale parallel electrical contacts[J]. Scientific Reports, 2019, 9(1): 1-14.



Behabtu, Natnael, et al. "Strong, light, multifunctional fibers of carbon nanotubes with ultrahigh conductivity." science 339.6116 (2013): 182-186.

- **Statistical analysis** can be performed by changing the contact length and gap distance using **Gaussian distributions** to compare with the experimental results.

II. Models



$$\bar{x}=\frac{x}{L},\ \bar{R}_{sh2}=\frac{R_{sh2}}{R_{sh1}},\ \bar{\rho}_c(\bar{x})=\frac{\rho_c(x)}{\rho_{c0}}$$

$$\bar{V}_1(\bar{x})=\frac{V_1(x)}{V_0},\ \bar{V}_g(\bar{x})=\frac{V_g(x)}{V_0},\ \bar{V}_2(\bar{x})=\frac{V_2(x)}{V_0}$$

$$\bar{I}_1(\bar{x})=\frac{I_1(x)}{I_0},\ \bar{I}_2(\bar{x})=\frac{I_2(x)}{I_0},\ \bar{J}_c(\bar{x})=\frac{J_c(x)LW}{I_0}$$

$$I_0=\frac{wV_0}{R_{sh1}L},\ R_{c0}=\frac{R_{sh1}L}{w},\ \bar{R}_c=\frac{R_c}{R_{c0}}$$

- **Transmission Line Model**

$$I_1(x)-I_1(x+\Delta x)=\frac{V_1(x)-V_2(x)}{\rho_c(x)}\Delta x\ \omega$$

$$V_1(x)-V_1(x+\Delta x)=I_1(x)\,R_{sh1}\Delta x/\omega$$

$$I_2(x+\Delta x)-I_2(x)=\frac{V_1(x)-V_2(x)}{\rho_c(x)}\Delta x\ \omega$$

$$V_2(x)-V_2(x+\Delta x)=I_2(x)\,R_{sh2}\Delta x/\omega$$

Normalize

$$\frac{\partial^2\bar{V}_1(\bar{x})}{\partial\bar{x}^2}=\bar{J}_c(\bar{x})$$

$$\frac{\partial^2\bar{V}_g(\bar{x})}{\partial\bar{x}^2}=(1+\bar{R}_{sh2})\bar{J}_c(\bar{x})$$

$$\bar{\rho}_c(\bar{x})\frac{\partial^2\bar{I}_1(\bar{x})}{\partial\bar{x}^2}+\frac{\partial\bar{\rho}_c(\bar{x})}{\partial\bar{x}}\frac{\partial\bar{I}_1(\bar{x})}{\partial\bar{x}}-(1+\bar{R}_{sh2})\bar{I}_1(\bar{x})+\alpha\bar{R}_{sh2}=0$$

$$R_c=\frac{V_0}{I_{tot}}$$

$$I_{tot}=\alpha I_0=\frac{\alpha wV_0}{Rsh1L}$$

$$R_c=\frac{Rsh1L}{\alpha w}$$

- **Tunneling Current Model**

Simmon's formular [1]:

$$\bar{J}_c=B\left(\overline{\varphi_I}e^{-A\Delta\bar{y}\sqrt{\overline{\varphi_I}}}-(\overline{\varphi_I}+\bar{V}_g)e^{-A\Delta\bar{y}\sqrt{\overline{\varphi_I}+\bar{V}_g}}\right)$$

$$\overline{\varphi_I}=\overline{\varphi_0}-\frac{\overline{y_1}+\overline{y_2}}{2}\bar{V}_g-\frac{1.15\bar{\lambda}}{\Delta\bar{y}}\ln\frac{\overline{y_2}(1-\overline{y_1})}{\overline{y_1}(1-\overline{y_2})}$$

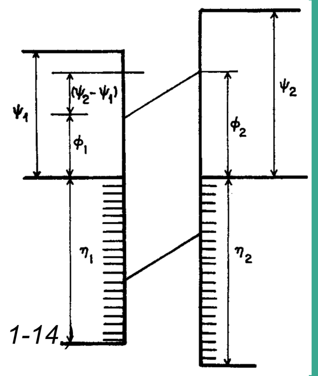
In CNT-vacuum-CNT parallel contact:
$\rho L=20k\Omega$, $w=3nm$, $Rsh1=Rsh2=60\Omega/square$, $W1=W2=4.5eV$, $\varepsilon_r=1.0$

For $\bar{V}_g\le\overline{\varphi_0}$

$$\overline{y_1}=\frac{1.2\bar{\lambda}}{\overline{\varphi_0}}\qquad \overline{y_2}=1-\frac{9.2\bar{\lambda}}{3\overline{\varphi_0}+4\bar{\lambda}-2\bar{V}_g}+\overline{y_1}$$

For $\bar{V}_g>\overline{\varphi_0}$

$$\overline{y_1}=\frac{1.2\bar{\lambda}}{\overline{\varphi_0}}\qquad \overline{y_2}=\frac{\overline{\varphi_2}-5.6\bar{\lambda}}{\bar{V}_g}$$



(The definition of the parameters are in Banerjee S, Luginsland J, Zhang P. , Scientific Reports, 2019, 9(1): 1-14.)

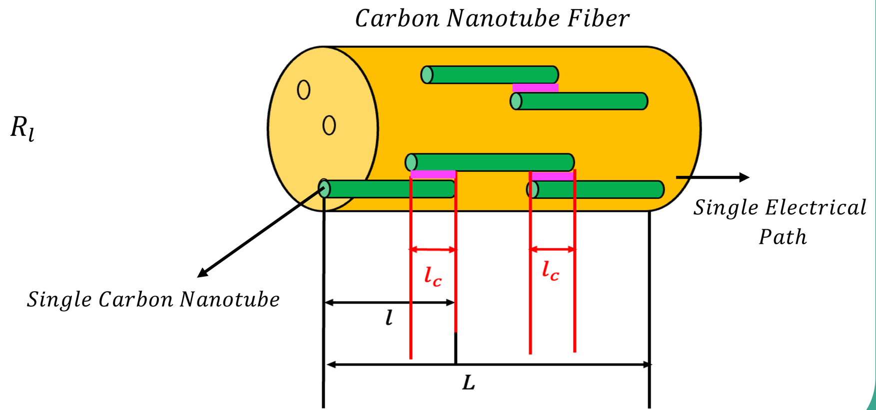
- **Macroscopic CNT Fiber Model**

$$2*(l-L_c)+(n-2)*(l-2L_c)+(n-1)*L_c=L$$

$$(n-2)*\rho_{CNT}\frac{(l-2L_c)}{A}+n*R_c+2\rho_{CNT}\frac{(l-L_c)}{A}=R_l$$

$$R_{CNF}=\frac{R_l}{N/n}$$

L_c(Overlap Length)[nm]	n(quantity of CNTs in single electrical path)
100	17006
300	17301
500	17605
700	17921

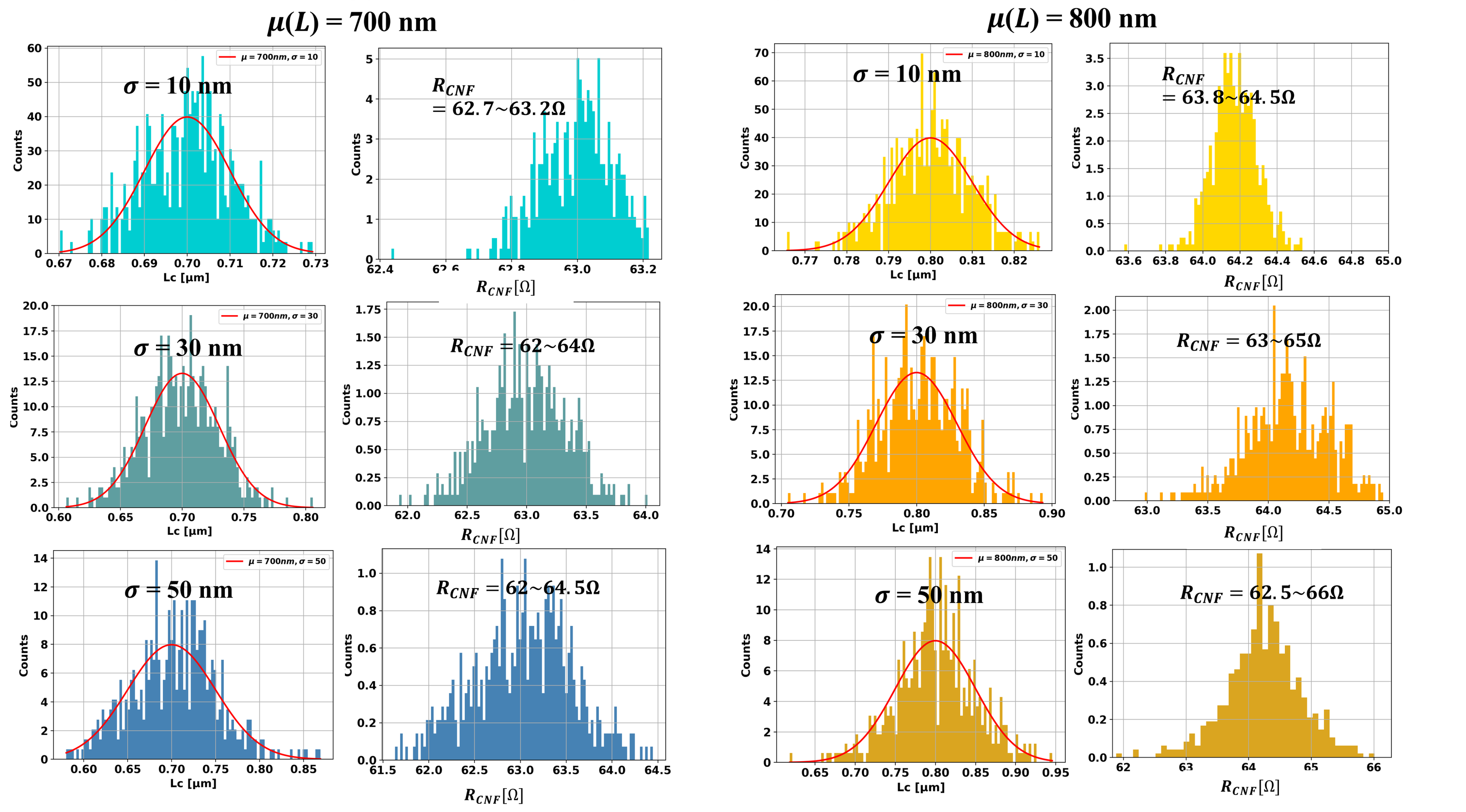


R_l is the resistance of single electrical path, N is the number of CNTs inside the CNT fiber ,

III.Gaussian Distribution of Parameters

Generates the **overlap length L_c** using Gaussian random number generator: $f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
$\left(\rho_{mCNT}=1.8\frac{g}{cm^3}\quad \rho_{mCNF}=1.6\frac{g}{cm^3},\sigma_{CNT}=1.3*10^6\frac{S}{m}\quad \sigma_{CNF}=7.7*10^6\frac{S}{m},L=0.2m\quad D=0.2\ \mu m.\ \ l=11.86\ \mu m.\ \ d=2.1\ nm,\ \text{double wall CNT}\right)$

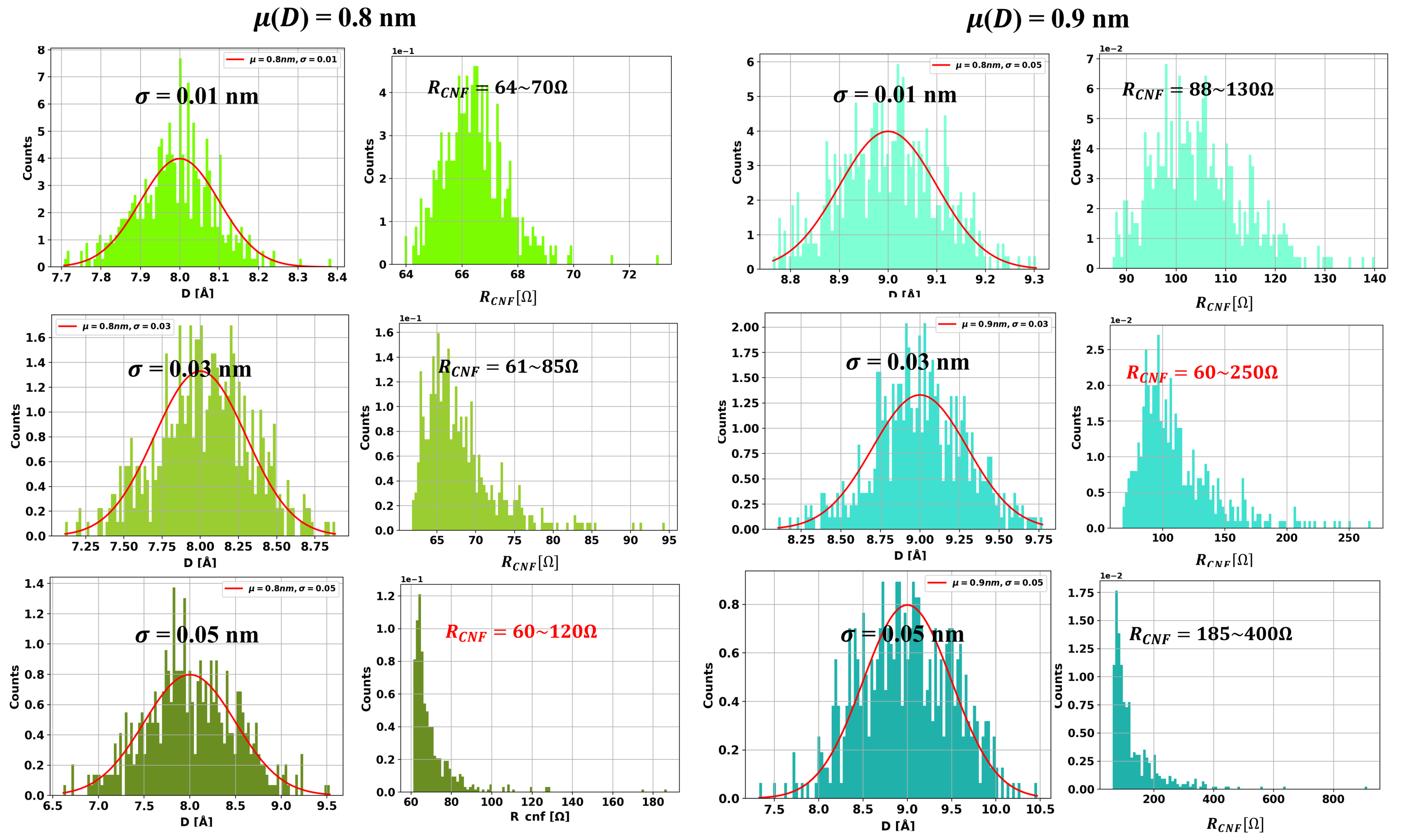
$\mu(L)=700$ nm / **$\mu(L)=800$ nm**



(For fixed gap distance $D=0.5nm$, μ is the mean value, σ is the standard deviation, $f(x)$ is the counts, the sample size is 500.)

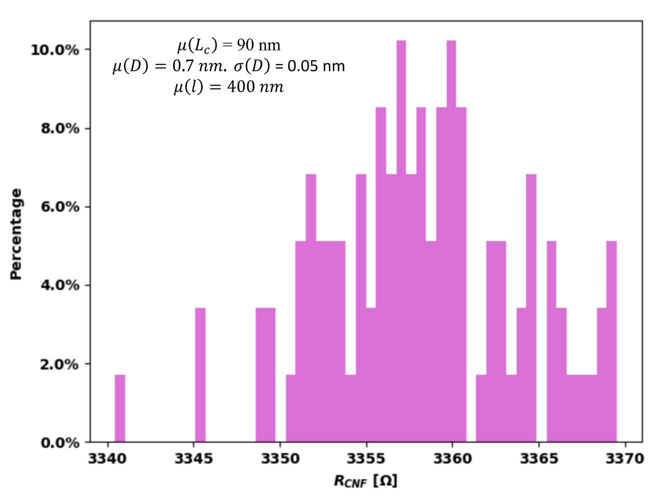
Generates the **Gap distance D** using Gaussian random number generator:

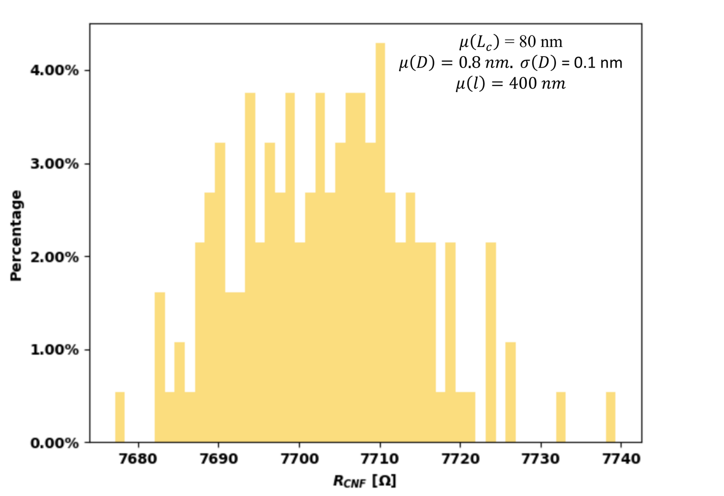
$\mu(D)=0.8$ nm / **$\mu(D)=0.9$ nm**



(For fixed overlap length $L_c=700\ nm$, μ is the mean value, σ is the standard deviation, f(x) is the counts, the sample size is 500.)

When the mean value of gap distance is $D=0.9\ nm$, and the overlap length is $L_c=700\ nm$, the distribution of the resistance of the CNT fiber is close to the experimental value (R_{CNF}= 82.72Ω for 0.2m long's fiber)(Using the parameters in Ref.[2])





Simultaneously vary the gap distance D, contact length L_c, and the length of an individual CNT l using Gaussian distributions. The resulting distributions of the CNT fiber resistance R_{CNF} for a sample size of 100,150 is shown. We assume that the length of CNT fiber is L = $20\mu m$, diameter is $0.1\mu m$.

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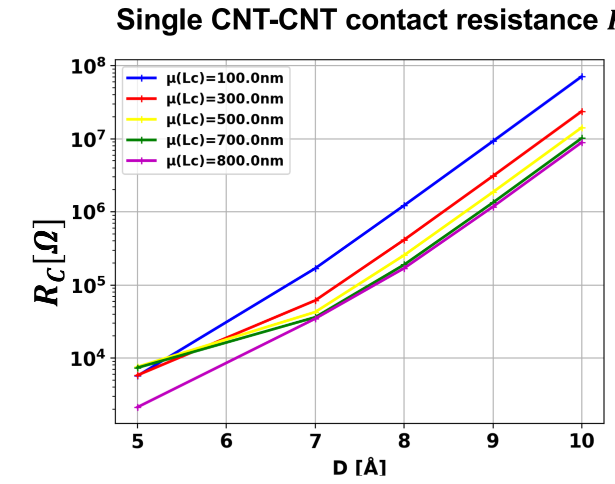
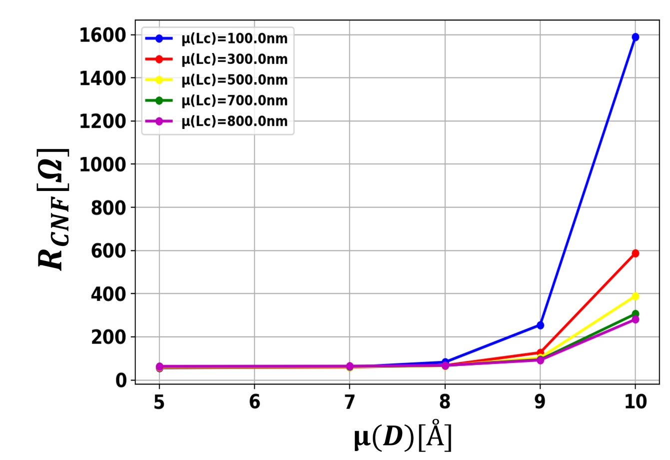
V. Effects of Gap Distance

Single CNT-CNT contact resistance R_c



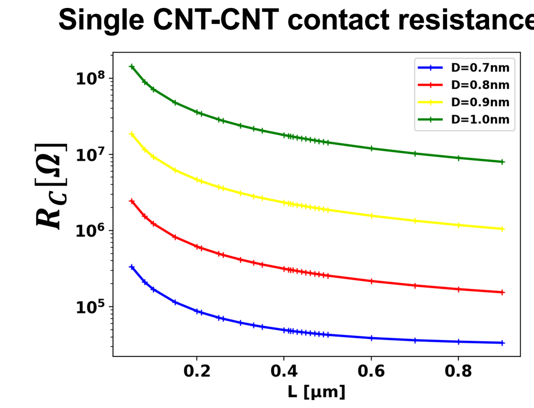
Macroscopic resistance of CNT fiber R_{CNF}



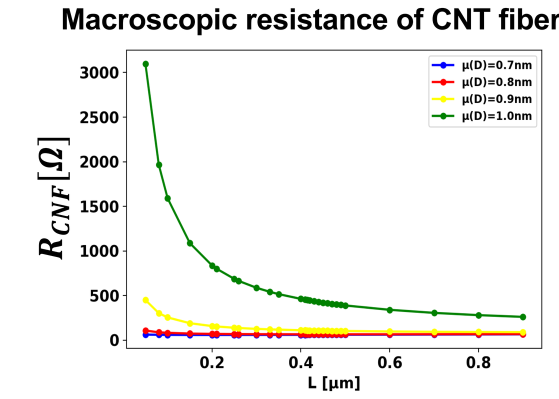
- The single CNT-CNT contact resistance R_c increases as the gap distance D increases
- When the mean value of gap distance $\mu(D)>0.8\ nm$, the macroscopic resistance of CNT fiber shows a stronger dependence on L_c

IV. Effects of Overlap Length

Single CNT-CNT contact resistance R_c



Macroscopic resistance of CNT fiber R_{CNF}



- The single CNT-CNT contact resistance R_c decreases as overlap length L_c increases for $D>0.5$ nm.
- When $L_c>200$ nm, macroscopic resistance of CNT fiber R_{CNF} increases as L_c increases for D < 1 nm (as the number of CNTs along the electrical path increases per unit length [Table on the left]).
- The macroscopic resistance of CNT fiber is more sensitive to the gap distance D than the overlap length L_c.

VI. Conclusion

- We analyzed the distribution of the resistance of CNT fiber with the Gaussian distribution of overlap length and gap distance to compare with the experimental values. Our model shows good agreement with experimental measurements, it may be used to investigate the electrical properties of CNT fibers. The standard deviation of gap distance affects the distribution of resistance strongly.
- Increasing the overlap length decreases the single CNT-CNT contact resistance, but increases the macroscopic resistance of CNT fiber (if the mass density of the CNF is fixed).
- Increasing the gap distance increases both single CNT-CNT contact resistance and CNT fiber resistance.

References

[1] Banerjee S, Luginsland J, Zhang P. , Sci. Rep. 9, 14484 (2019).
[2] Tsentalovich, Dmitri E., et al. Macromolecules 49.2 (2016): 681-689.
[3] Tsentalovich, Dmitri E., et al. ACS applied materials & interfaces 9.41 (2017): 36189-36198.

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