

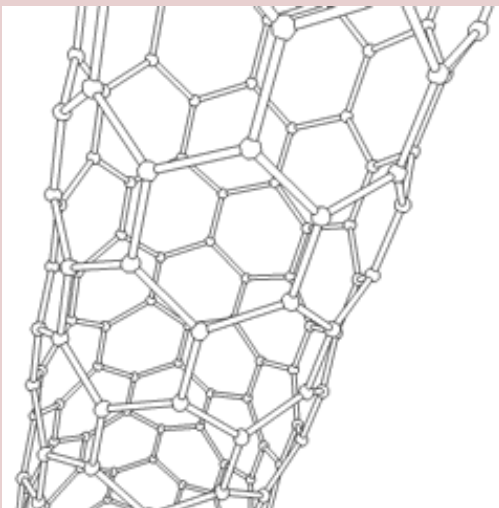
# Computer Modeling and Design of Carbon Nanotube Embedded MOS Chemicapacitive Sensors

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## Carbon Nanotube:



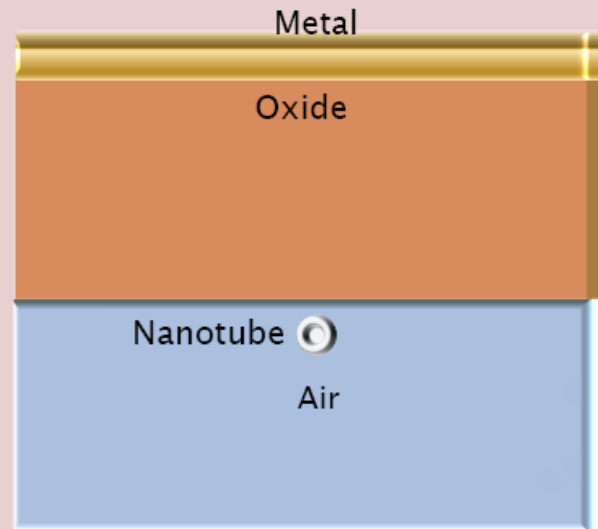
Schwarzsm. (30 August 2004). Carbon nanotube.

August 1 2006, Available:

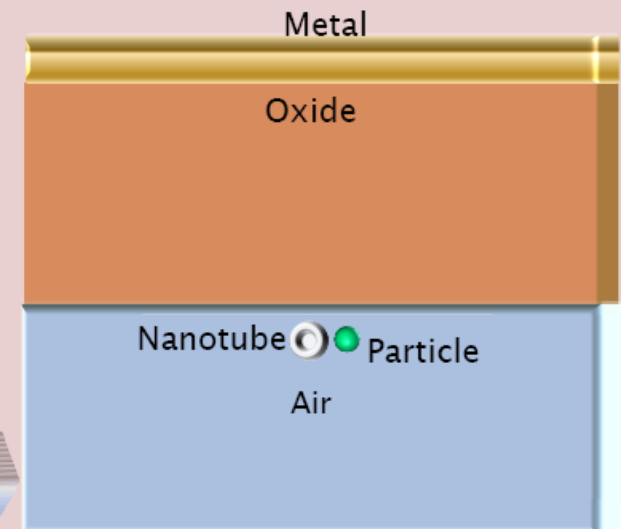
[http://commons.wikimedia.org/wiki/Image:Kohlenstoffnanorohre\\_Animation.gif](http://commons.wikimedia.org/wiki/Image:Kohlenstoffnanorohre_Animation.gif). Used under GNU FDL

## Our Proposed Sensor Design:

Clean:



Contaminated:



- We aim to simulate a nanotube-embedded device able to detect small chemical and biochemical particles with a high sensitivity and quick response rate.
- Such a device will help to mitigate the risk of environmental contamination harming soldiers, an unfortunate tactic that has been a feature of warfare for thousands of years.

- To study the electrostatic properties of the sensor, we solve the **Poisson Equation** for  $\phi : \nabla \cdot (\epsilon \nabla \phi) = -q\rho$  where

$\phi$  is the electrostatic potential;  $\epsilon$  is the dielectric constant;  
 $\rho$  is the net charge density;  $q$  is the electronic charge

- Interface equation (all nonuniform meshes):

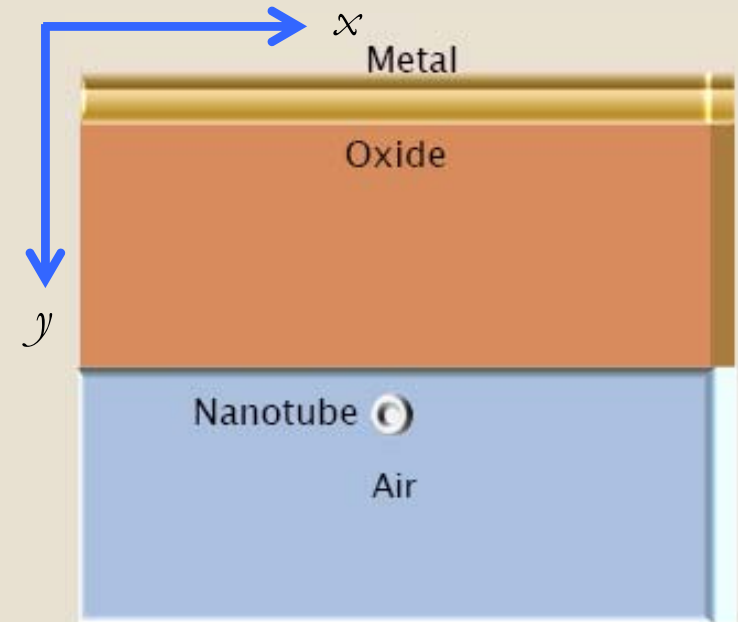
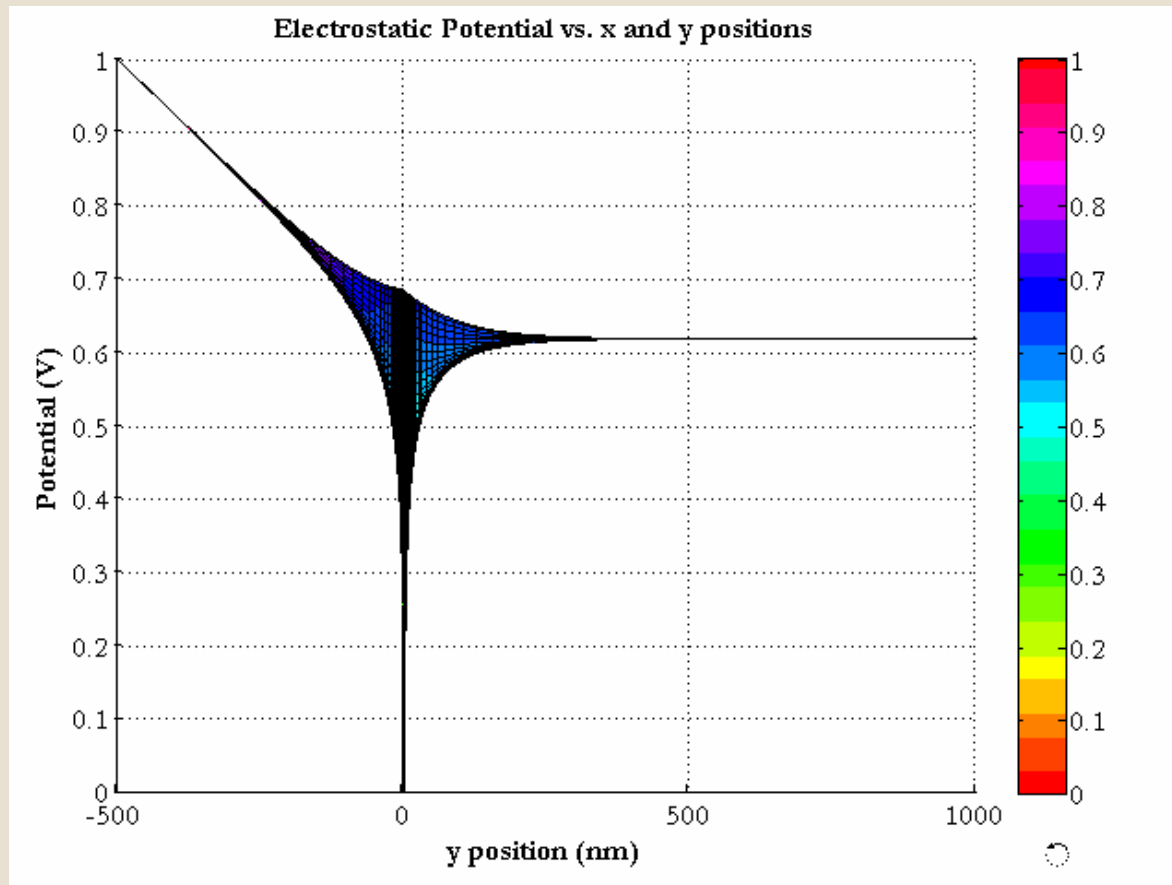
$$\frac{\epsilon_{oxide}}{\Delta_y(j-1)} \phi(y_0 - \Delta_y(j)) - \left( \frac{\epsilon_{oxide}}{\Delta_y(j-1)} + \frac{\epsilon_{air}}{\Delta_y(j)} \right) \phi(y_0) + \frac{\epsilon_{air}}{\Delta_y(j)} \phi(y_0 + \Delta_y(j)) = 0$$

- Two dimensional nonuniform mesh numerical approximation equation:

$$\begin{aligned} & \frac{2}{\Delta_y(j-1)(\Delta_y(j) + \Delta_y(j-1))} \phi \begin{pmatrix} x \\ y - \Delta_y(j) \end{pmatrix} + \frac{2}{\Delta_x(i-1)(\Delta_x(i) + \Delta_x(i-1))} \phi \begin{pmatrix} x - \Delta_x(i) \\ y \end{pmatrix} \\ & - \left( \frac{2}{\Delta_x(i-1)\Delta_x(i)} + \frac{2}{\Delta_y(j-1)\Delta_y(j)} \right) \phi \begin{pmatrix} x \\ y \end{pmatrix} \\ & + \frac{2}{\Delta_x(i)(\Delta_x(i) + \Delta_x(i-1))} \phi \begin{pmatrix} x + \Delta_x(i) \\ y \end{pmatrix} + \frac{2}{\Delta_y(j)(\Delta_y(j) + \Delta_y(j-1))} \phi \begin{pmatrix} x \\ y + \Delta_y(j) \end{pmatrix} = 0 \end{aligned}$$

# Solution for Potential

- Overview of potential with 2 nm by 2 nm nanotube embedded in MOS:

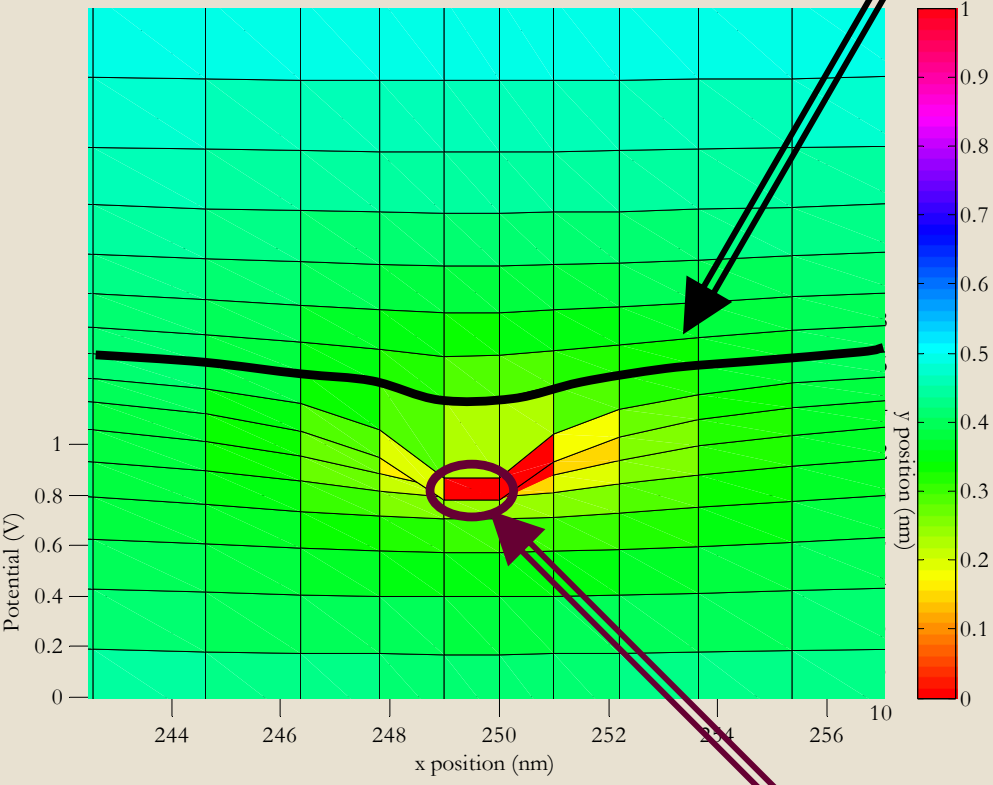


# Zoom In on Potential

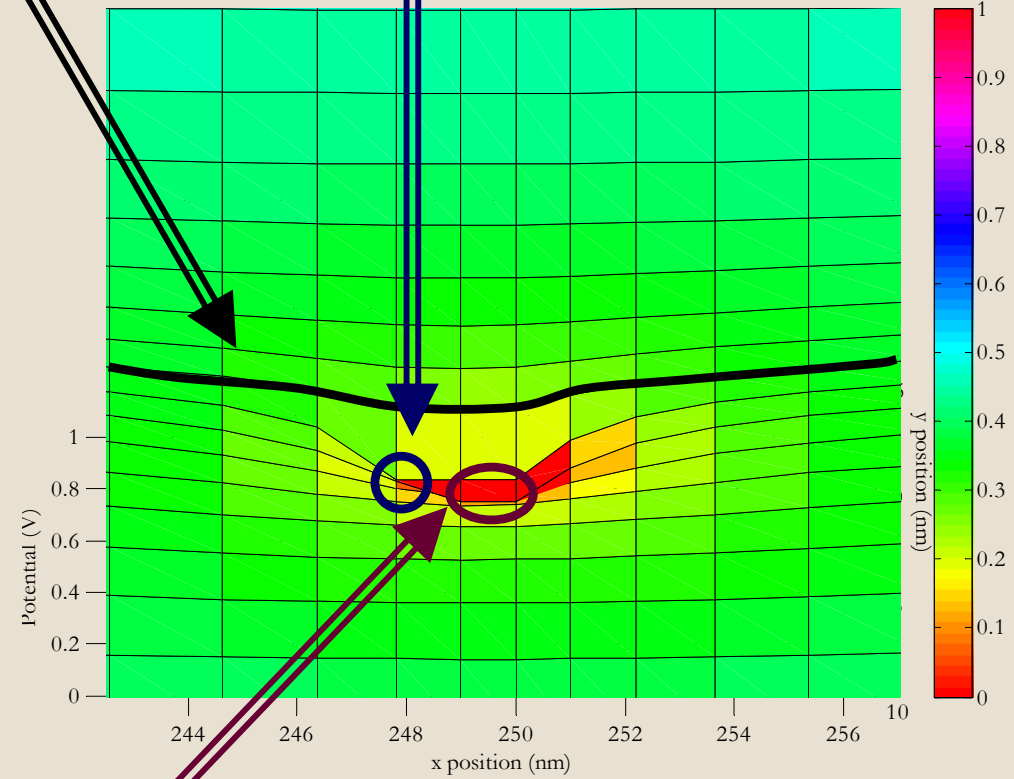
Interface

Fixed potential representing particle

Electrostatic Potential vs. x and y positions



Electrostatic Potential vs. x and y positions



Fixed potential representing nanotube

# Analysis and Conclusions

- The numerical solutions show unequivocally that the proposed design for a nanotube sensor is advantageous over the traditional design in terms of sensitivity upon the insertion of a particle.

