4. NANO-ELECTROMAGNETIC COMPUTATION AND APPLICATIONS OR
9. COUPLED MULTI-PHYSICS PROBLEMS

Numerical Modeling of Joule Heating in a Single Carbon Nanotube during Electron Field Emission

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Abstract —Resistive heating on a single carbon nanotube (CNT) due to electron field emission is investigated in details using a combination of customized classic heat equations and numerical techniques. The static electric field is evaluated using the finite element method and the emission current and temperature of the CNT is modeled analytically. A more up to date field enhancement factor for CNT is applied to a classic temperature model yielding results that are in good agreement with experiments described by other authors. The effects of the temperature on the I/V curves for field emission in CNT are investigated.

I. Introduction

The potential of carbon nanotubes (CNT) as an electron field emitter source that requires a low electric field magnitude to create high current densities are acknowledged today [1-5]. Field emission (FE) applications for CNT are numerous and its arrangement is often classified in single or multiple electron beam devices. A promising application of a single electron beam apparatus is an electron microscope using one nanotube as a FE electron source to create a very coherent electron beam [6]. Flat panel display is a recognized example where an arrangement of CNT´s provides a large number of independent electron beam sources that address each pixel on the display [2]. For applications where CNT is used as a current carrying conductor, it is important to understand the Joule heating behavior as this characterizes important limits, especially in situations with high current densities as in FE.

II. Numerical Model and Field Emission Theory

The calculation of the electric field, current density, field emission current and temperature were all done using the commercial code Ansys Maxwell that uses the finite element method as basis. We have created a 3D CNT model based on a classic 2D cylinder-shaped geometry [6,7]. The model is comprised of an anode where the voltage required to generate the field is applied and a cathode which is grounded and connected to the CNT. The 3D model was developed because it allows the simulation of any arbitrary geometry.

In order to perform an electrostatic analysis, and assuming the absence of charge-space effects, the electric potential distribution Φ is evaluated using the following 2D Laplace equation:

$$\nabla^2\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} = 0 \tag{1}$$

The electric field distribution is then calculated by numerically differentiating the potential distribution with respect to x and y Cartesian coordinates. Figure 1 shows a scaled model of voltage and electric field plot, where a 100V excitation was applied to the anode while the CNT and the cathode was kept grounded.

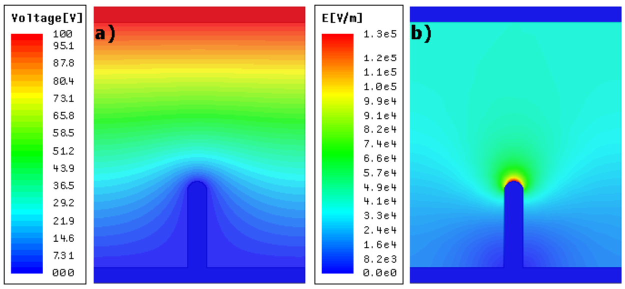

Fig. 1. Cross sectional plots: a) Voltage [V] and b) Electric field [V/m]

The electric field is natively calculated by the software Ansys Maxwell and in order to compute the current density one need to use the Fowler-Nordheim (FN) theory. The common form of the current density $J(E)$ as a function of the electric field E is given by equation 2 [8]:

$$J(E) = \frac{AE^2}{\phi t^2(y)} \exp\left(-\frac{B\phi^{3/2}v(y)}{E}\right) \tag{2}$$

where ϕ is the CNT work function and

$$\begin{aligned} &A_1(\phi) = \left(\frac{A}{\phi}\right)\exp\left(\frac{By_0^2}{\sqrt{\phi}}\right); \\ &E_C(\phi) = Bv_0\phi^{3/2};\ v(y) = 0.95 - y^2; \\ &y = 3.7\times10^{-4}\sqrt{E/\phi};\ A = 1.5\times10^{-6};\ B = 6.8\times10^{7}; \end{aligned} \tag{3}$$

The field emission current I_{FE} can be calculated by integrating the current density over the CNT surface.

$$I_{FE} = \iint_{CNT} J(E)dS \tag{4}$$

Equations 2- 4 are used to evaluate the I_{FE} of field emitters and CNT's. Nevertheless, the same formulations disregard current induced heating.

III. Joule Heating Model

Assuming that the thermal conductivity and resistive heating are the main energy exchange processes during field emission, one can use the general heat conduction equation in spherical polar coordinates to analyze the temperature rise on the CNT [9]:

$$\frac{\partial T}{\partial t}=\frac{K}{\sigma S}\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 T}{\partial\theta^2}\right] \quad (5)$$

where r is the CNT tip radius, S is the CNT specific heat, and σ is the Stefan–Boltzmann Constant**.** When $\partial T/\partial t=0$, temperature as a function of the current density can be calculated using the following equation [6]:

$$J(E)^2 r^2=\frac{2KT}{\rho(\beta-2)^2} \quad (6)$$

where ρ is the mean resistivity, K is the mean thermal conductivity and β is the field enhancement factor. The classic model of equation 6 uses the field enhancement factor $\beta=(L/r)+2$ where L is the CNT length [6]. We can replace β in our model for a more accurate and up to date field enhancement factor [7] resulting in equation 7:

$$J(E)^2 r^2=\frac{2KT}{\rho\left[1.2(L/r+h)^c-2\right]^2} \quad (7)$$

The dimensions of the model was based on experimental CNT dimensions [10] with L=40µm, r=10nm and s=100µm as show schematically in the inset of figure 2. After rearranging equation 7 it is possible to determine the temperature on the CNT surface:

$$T=\frac{J(E)^2 r^2\rho\left[1.2(L/r+2.15)^{0.90}-2\right]^2}{2K} \quad (8)$$

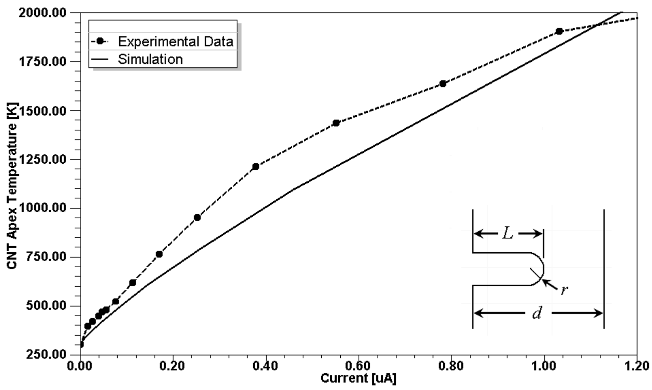

Fig 2. Maximum CNT temperature as a function of the field emission current.

The dependence of the CNT properties with its growing process is very high. We have considered the following properties for our simulations [11]: $K=100$ *W/(mK)*, $\rho=3.2\times10^{-5}$ Ωm and $\phi=5.1$ *eV*. The highest temperature is found at the apex of the CNT, T_A, due to the current density in this particular region. Figure 2 shows a comparison between the T_A values obtained experimentally [12] and through simulation. The temperature visualization on the CNT surface is observed in figure 3. This plot is useful for a better visualization of the phenomenon and it can be generated since we are using a 3D model.

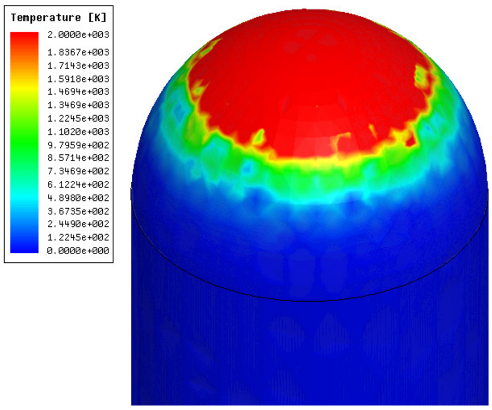

Fig 3. 3D temperature plot on the CNT surface.

IV. CONCLUSIONS

A numerical study of the field emission in CNT including resistive heating effects was demonstrated. We have proposed an update in a classic heating model by replacing the field enhancement factor with a more accurate function. This enables the temperature calculation and its effects to be included in the emission current analysis in a more precise way using only one electromagnetic code: Ansys Maxwell. Results indicate that the mathematical procedure presented in this paper is in good agreement with experimental results reported in the literature.

V. REFERENCES

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