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Proceedings in Applied Mathematics and Mechanics (PAMM),
Wiley, Vol. 71 (1)
(Special Issue: Sixth ICIAM and GAMM Annual Meeting, Zurich),
pp. 1030801-1030802, 2008.

Editor: Gesellschaft für Angewandte Mathematik und Mechanik (GAMM)

Online ISSN:1617-7061

Wiley-VCH GmbH, Weinheim

PAMM Proceedings in Applied Mathematics and Mechanics

PAMM · Proc. Appl. Math. Mech. **7**, 1030801–1030802 (2007) / **DOI** 10.1002/pamm.200700034

Coupled nonlinear effects in modeling field emission from CNTs

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Field emission from carbon nanotubes (CNTs) is a complex process involving a range of physical effects and phenomena. In this paper, we systematically develop a multiphysics model to describe this process. We integrate the model numerically to estimate the output current from a CNT based field emission device. Numerical simulations have been able to capture the transients in current as observed in actual experiments.**

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1 Introduction

Technologically proven methods for electron emission are mostly thermionic in nature, where electrons are emitted from heated filaments. However, thermionic cathodes have slow response time and limited lifetime due to mechanical wear. In addition, these cathodes consume high power and the emitted electrons have random spatial distribution. This adversely affects the performance of devices such as x-ray tubes because fine focussing of electron beam becomes very difficult. An alternative to extract electrons is field emission. It is due to a quantum-mechanical effect where the electrons near the Fermi level tunnel through the energy barrier and escape to the vacuum under the influence of external electric field. There are several advantages of selecting a field emitting cathode over a thermionic one: (i) current density from field emission would be orders of magnitude greater than in the thermionic case, (ii) a cold cathode would minimize the need of cooling, and (iii) a field emitting cathode can be miniaturized. Due to their improved spatial and temporal resolution, field emission x-ray sources can also be used for imaging of skeletal structures. It has been reported that carbon nanotube (CNT) based x-ray sources, which utilize field emission mechanism, can generate diagnostic quality x-rays [1]. In such x-ray sources, the cathode comprises of an ensemble of CNTs. This ensemble undergoes complex dynamics during field emission, which includes processes such as evolution and electromechanical interactions. Such processes, which are coupled and nonlinear, must be analyzed accurately from the view-point of stable and long-term performance of the device. In this paper, we have developed a mechanics-based model for electromechanical interactions among CNTs during field emission, which is employed for calculating the strain and displacement in CNTs. These quantities are coupled with the electric field for estimating the output current by employing a semi-empirical Fowler-Nordheim (FN) equation.

2 Mathematical model

The physics of field emission is fairly well understood, where the current density (J) is usually obtained by using the FN equation [2]: $J = (BE^2/\Phi)\exp(-C\Phi^{3/2}/E)$; E is the electric field, Φ is the work function of the cathode material, and B and C are constants. The phenomenological model of evolution of CNTs is given by four nonlinear coupled ordinary differential equations [3]. Based on this model, the rate of degradation of CNTs ($v_{\rm burn}$) and the effective electric field component (E_z) for field emission calculation are defined as, respectively,

$$v_{\rm burn} = V_{\rm cell}\frac{dn_1(t)}{dt}\left[\frac{s(s-a_1)(s-a_2)(s-a_3)}{n^2a_1^2+m^2a_2^2+nm(a_1^2+a_2^2-a_3^2)}\right]^{1/2}, \quad E_z = \sqrt{1-\frac{x^2+y^2}{R^2}}\,\frac{(h_0-v_{\rm burn}t)E_0}{(d-h_0+v_{\rm burn}t)}\cos\theta(t)\ , \quad (1)$$

where $V_{\rm cell}$ is the representative volume element, n_1 is the concentration of carbon atoms in the cluster form in the cell, t is the time, a_1, a_2, a_3 are lattice constants, $s = \frac{1}{2}(a_1+a_2+a_3)$, n and m are integers ($n \geq |m| \geq 0$) that define the chirality of the CNT, x and y are the deflections of the tip with respect to its original location, 2R is the spacing between two adjacent CNTs at the cathode substrate, h_0 is the initial average height of the CNTs, d is the distance between the cathode substrate and the anode, $E_0 = V/d$ with V being the applied DC voltage, and $\theta(t)$ is the tip orientation angle that a CNT makes with the Z-axis. In order to account for the changing orientations of CNTs, electromechanical forces have been modeled by the authors [4]. Next, we employ these force components ($f_{x'}$, $f_{z'}$), which are defined in the local (X', Z') coordinate system, in the expression of work done on the ensemble of CNTs and formulate an energy conservation law. Due to their large aspect ratio, the CNTs have been idealized as one-dimensional elastic members (as for Euler-Bernoulli beams). By introducing the

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** The text of the Abstract is changed compared to a prior version.

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strain energy density, the kinetic energy density and the work density, and applying the Hamilton principle, we obtain the governing equations in $(u_{x'}, u_{z'})$ for each CNT, which can be expressed as

$$E'A_2\frac{\partial^4 u_{x'}}{\partial z'^4} + \rho A_0 \ddot{u}_{x'} - \rho A_2 \frac{\partial^2 \ddot{u}_{x'}}{\partial z'^2} - f_{x'} = 0 \ , \quad -E'A_0\frac{\partial^2 u_{z'0}}{\partial z'^2} - \frac{E'A_0\alpha}{2}\frac{\partial \Delta T(z')}{\partial z'} + \rho A_0 \ddot{u}_{z'0} - f_{z'} = 0 \ , \quad (2)$$

where $u_{x'}$ and $u_{z'}$ are lateral and longitudinal displacements of the oriented CNTs, E' is the effective modulus of elasticity of CNTs, A_2 is the second moment of cross-sectional area about Z-axis, A_0 is the effective cross-sectional area, ρ is the mass per unit length of CNT, $\Delta T(z') = T(z') - T_0$ is the difference between the absolute temperature (T) during field emission and a reference temperature (T_0), and α is the effective coefficient of thermal expansion (longitudinal). We assume fixed boundary conditions ($u = 0$) at the substrate-CNT interface ($z = 0$) and forced boundary conditions at the CNT tip ($z = h(t)$).

By considering the Fourier heat conduction and thermal radiation from the surface of CNT, the energy rate balance equation in T can be expressed as

$$dQ - \frac{\pi d_t^2}{4} dq_F - \pi d_t \sigma_{SB}(T^4 - T_0^4)dz' = 0 \ , \quad (3)$$

where dQ is the heat flux due to Joule heating over a segment of a CNT, q_F is the Fourier heat conduction, d_t is the diameter of the CNT and σ_{SB} is the Stefan-Boltzmann constant. First, the electric field at the nodes are computed, and then all the governing equations are solved simultaneously at each time step and the curved shape $s(x' + u_{x'}, z' + u_{z'})$ of each of the CNTs is updated. The angle of orientation θ between the nodes $j+1$ and j at the two ends of segment Δs_j is expressed as

$$\theta(t) = \tan^{-1}\left(\frac{(x^{j+1} + u_x^{j+1}) - (x^j + u_x^j)}{(z^{j+1} + u_z^{j+1}) - (z^j + u_z^j)}\right) \ , \quad \begin{bmatrix} u_x^j \\ u_z^j \end{bmatrix} = [\Gamma(\theta(t - \Delta t)^j)] \begin{bmatrix} u_{x'}^j \\ u_{z'}^j \end{bmatrix} \ , \quad (4)$$

where Γ is the usual coordinate transformation matrix which maps the displacements $(u_{x'}, u_{z'})$ defined in the local (X', Z') coordinate system into the displacements (u_x, u_z) defined in the cell coordinate system (X, Z).

3 Results and discussions

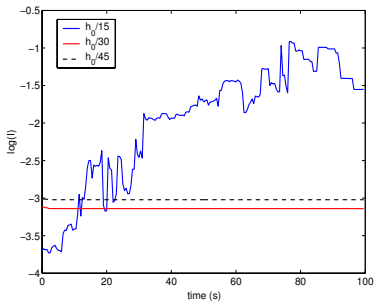

Fig. 1 Representative field emission current histories for various initial average tip deflections and under bias voltage of 650V. See [4] for details.

The CNT film considered in this study consists of randomly oriented multiwalled CNTs grown on a stainless steel substrate. The orientation of CNTs is parametrized in terms of the upper bound of the CNT tip deflection (denoted by h_0/m', $m' >> 1$). The current history is simulated as in [4] with variation in few parameters. Several computational runs are performed and the output data are averaged out at each sampling time step. For a constant bias voltage ($650V$ in this case), as the initial state of deflection of the CNTs increases (from $h_0/45$ to $h_0/15$), the average current reduces until the initial state of deflection becomes large enough that the electrodynamic interaction among CNTs produces sudden pull in the deflected tips towards the anode resulting in current spikes (see Fig. 1).

4 Conclusions

In this paper, a model has been developed, which sheds light on nonlinearities and coupling issues related to the electrodynamics, the mechanics, and the thermodynamics during the process of field emission from CNTs in a thin film. The proposed modeling approach handles several complexities at the device scale. This model can be useful in designing the CNT pattern for the development of x-ray devices for precision biomedical instrumentation.

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