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Theoretical Investigations of the Effect of N-Doping on Growth and Field Emission Properties of Carbon Nanotubes (CNTs)

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Abstract. In this work, we investigate effects of doping of hetero-atoms such as Nitrogen (N) on the growth and field emission properties of Carbon Nanotubes (CNTs) in low temperature plasma. A theoretical model is developed to incorporate kinetics of electron, ions and neutral atoms with N as dop ing elements in complex and low temperature plasma. Results of numerical calculations of the radius of N-doped CNT are presented for typical glow discharge plasma parameters. It is found that the radius of CNT is reduced with N-doping. The field enhancement factor of CNT is also estimated from the obtained results.

1. Introduction

The effect of the experimental parameters on the structure of nitrogen containing Multi-Wall Nanotubes (MWNTs) produced by an aerosol assisted Chemical Vapor Deposition (CVD) method has been studied by Koos *et al.* [1] previously. Ayala *et al.* [2] have demonstrated the effect of doping of carbon nanotubes with nitrogen. Kim *et al.* [3] have shown in their investigations that enhanced CNT growth in an N_2 or NH_3 environment is due to nitrogen incorporation into the CNT wall. Sharma and Tewari [4] have investigated the effect of plasma parameters on the growth and field emission properties of Carbon Nanotubes. The variation of field enhancement factor has been experimentally verified by Srivastava et al. [5] who also studied the enhanced field emission characteristics of nitrogen-doped carbon nanotube films showing field emissions at a level of 2.65–3.55 V/μm.

2. Model

Plasma containing electrons, positively charged ions of type *A*, B, and *C*, and neutral atoms of type *A*, *B*, and *C*, is considered. Here *A* corresponds to carbon, *B* to neon, and *C* to nitrogen as doping material. The initial radius of spherical CNT tip, r_0 , can be estimated by evaluating the accumulation of electrons and positively charged ions on the CNT,

$$n_e\left(\frac{T_e}{m_e}\right)^{\frac{1}{2}}\exp\left(-\frac{e^2}{r_0k_BT_e}\right)=\left(1+\frac{e^2}{r_0k_BT_i}\right)\left[n_{iA}\left(\frac{T_i}{m_{iA}}\right)^{\frac{1}{2}}+n_{iB}\left(\frac{T_i}{m_{iB}}\right)^{\frac{1}{2}}+n_{iC}\left(\frac{T_i}{m_{iC}}\right)^{\frac{1}{2}}\right], \quad (1)$$

with n_e and T_e the electron density and temperature, respectively. The ion temperature is denoted by T_i, the Boltzmann constant by k_B , and the electron charge by e. The densities of the ions are indicated by n_{iA} , n_{iB} and n_{iC} with masses m_{iA} , m_{iB} and m_{iC}, respectively.

2.1 Growth rate equation for the mass of CNT

The growth rate is evaluated using

$$\frac{d}{d\tau} m_{ct} = (m_A \gamma_A n_{Act} + m_{iA} \gamma_{iA} n_{iAct} + m_C \gamma_C n_{Cct} + m_{iC} \gamma_{iC} n_{iCct}) \, , \quad (2)$$

where m_{ct} is the mass of the CNT of radius a. With the density of the CNT, ρ_{ct}, the mass of the CNT can be expressed in terms of the density $m_{ct}=4/3\ \pi\ r^3\ \rho_{ct}$. The sticking coefficients for the atomic and ionic species are γ_A , γ_{iA} , γ_C and γ_{iC}, respectively. The two terms in Equation (2) correspond to gains in mass due to collection of atomic and ionic species A and C.

3. Results and discussion

For the developed model, calculations are carried out by taking the same parameters for the undoped spherical CNT tip as taken by Sharma and Tewari [4]. Calculations are for doped-nitrogen CNTs using boundary conditions and parameters at τ=0, n_{ct} =10^6 cm^{-3}, n_{iA0}=n_{iB0}=n_{iC0}=10^9 cm^{-3}, n_{A0}=n_{B0}=5×10^8 cm^{-3}, n_{C0}=5×10^8 cm^{-3}, n_{e0}=10^9 cm^{-3}, T_{e0}=0.5 eV, T_{i0}= 2500K, T_{n0}=T_{ct}=2000K. Further, $m_{iA} \approx m_A$=12 amu (carbon), $m_{iB} \approx m_B$=20 amu (neon) and $m_{iC} \approx m_C$=14 amu (nitrogen).

Figure 1 illustrates the variation of normalized radius r/r_0 of spherical CNT tip with time for undoped CNTs and nitrogen-doped CNTs. The value of normalized radius is found to be more for undoped CNTs, and it reduces with N-doped CNTs. This confirms better field emission for N-doped CNTs. Fig. 2 illustrates the variation of field enhancement factor for undoped and N-doped CNTs. The field enhancement factor, β, for N-doped CNTs has been calculated. The results show higher value of β for N-doped CNTs.

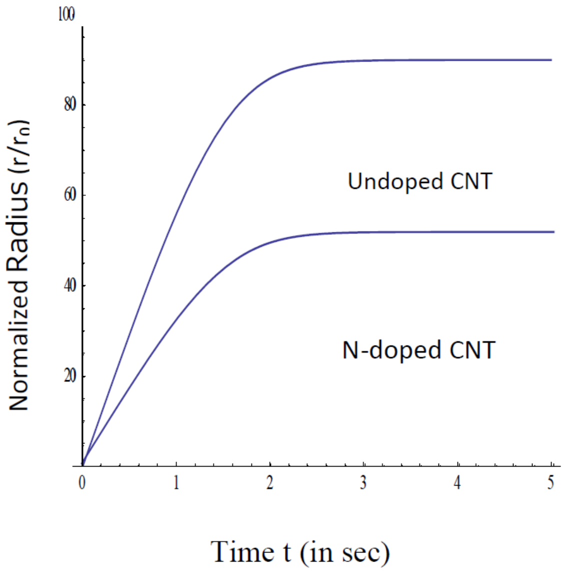

Figure 1. Variation of the normalized radius r/r_0 for undoped and N-doped CNTs.

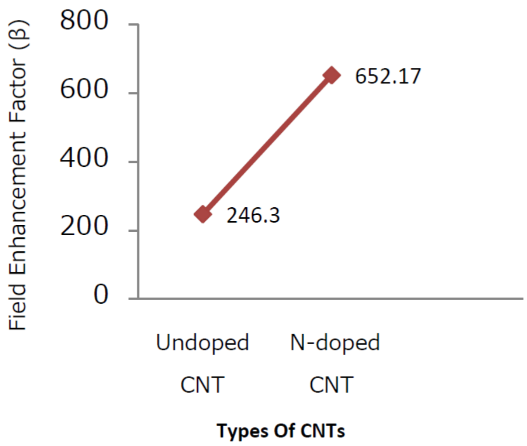

Figure 2. Variation of the field enhancement factor for undoped and N-doped CNT's.

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4. Conclusions

The model developed for calculating the growth of spherical CNT tip with nitrogen as doping material predicts a diminished radius with nitrogen-doped as compared to undoped CNTs. Moreover, the computed field enhancement factors β for both doped and undoped CNTs show a maximum value on the order of 650 for nitrogen–doped CNTs. The obtained results have also been experimentally verified by Srivastava *et al.* [5].

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