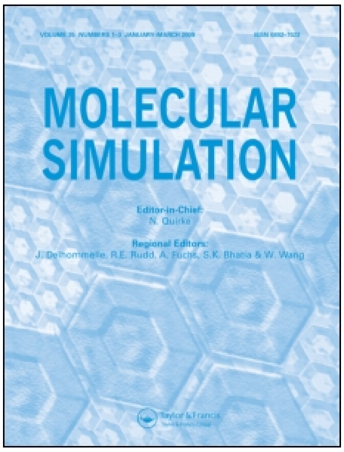

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Electron Field Emission from Carbon Nanotubes: Modeling and Simulations

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Electron Field Emission from Carbon Nanotubes: Modeling and Simulations

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Here, we present theoretical investigations on field emission properties of open and closed single-walled carbon nanotubes. These investigations include studies on the effects of geometry and electronic structure of the nanotubes. The electric field intensity and its spatial variation near the tips of open and closed nanotubes are calculated. The field intensity of an open nanotube in very close proximity of the tip is found to be higher but it decreases more rapidly with the distance. It is found that calculated emission currents from closed nanotubes are higher than that of open nanotubes at low electric fields. Emissions patterns are simulated and they are found to be related to the local electronic structure of the nanotube caps.

Keywords: Carbon nanotubes; Field emission; Modeling; Single-walled carbon nanotubes

INTRODUCTION

Carbon nanotubes have novel electronic and mechanical properties and they are promising materials for future technological applications. One of these possible future applications is using carbon nanotubes as electron field emitters. Using sharp tips such as carbon nanotubes as field emission materials creates the potential advantage of having very high brightness in a thin profile in display applications. The advantage of sharp tips is the enhancement of a local electric field at the apex of the tip to obtain high electron current density at modest device voltages. Carbon nanotubes offer the realization of atomic scale tips with their small diameters and high aspect ratios. Recent experiments have shown that nanotubes have excellent field emission properties with high current density at low electric fields [1–9]. On the other hand, fundamental understanding of the mechanisms of electron field emission from nanotubes is crucial. Here, we present theoretical investigations on the electron field emission properties of single-walled carbon nanotubes (SWNTs). These investigations include effects of both the geometrical and the electronic structure of nanotubes.

Field emission is a quantum mechanical tunneling problem that has been extensively studied since the late 1920s. It can be described as emission of electrons from surfaces by high electric fields and/or at high temperatures. Fowler and Nordheim developed a general model for electron emission from planar surfaces and their model has been widely used for electron emission from large objects. According to the Fowler–Nordheim model, emission from planar or large surfaces produces straight lines in so-called Fowler–Nordheim (F–N) plots (i.e. a $\log(I/V^2)$ vs. $1/V$). On the other hand, experimental F–N plots for nanotube field emitters deviate from straight lines [10]. In order to understand this behavior and the field emission mechanisms of nanotubes, a model that takes geometric and electronic nature of the nanotube into account is used. In the second section, the the model used to study field emission is described and in the third section, the results for open and closed nanotubes are presented.

MODEL

In order to study the electron field emission from SWNTs, a model that incorporates the geometry

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and electronic structure of nanotubes is used [11]. To determine the spatial variation of the electric field, Laplace's equation is solved numerically. The effective electronic potential is calculated using SCF-Pseudopotential electronic structure calculation method, and the variation of the local potential energy is obtained. Complete pseudopotentials given in the Kleinman–Bylander form [12,13] and the Ceperley–Adler [14] exchange-correlation potential are used in the electronic structure calculations. Localized electronic states at the nanotube cap are found to be very important for field emission [15,16]. The electronic structure of a nanotube is derived using a π-orbital tight-binding Hamiltonian [17]. Although only a finite region of the nanotube is under a high electric field, its electronic structure is similar to a very long or a semi-infinite nanotube. The surface Green's function matching method [18,19] is used on one end. Thus, nanotubes are considered to be semi-infinitely long for their electronic structure and the effects of finite lengths on the nanotubes' electronic structure are avoided. On the other hand, a finite portion of a nanotube including its cap is considered in the applied electric field region and will be referred to as the nanotube length. In addition, current-voltage characteristics for different tube sizes and lengths were calculated using the WKB approximation [20,21]. Using these methods, the effects of geometry and electronic structure on the field emission current are investigated.

RESULTS AND DISCUSSION

Recent experiments [22] and theoretical investigations [11] show that electric field is dramatically enhanced near the nanotube cap with a large variation of the local field distribution. This is due to the high aspect ratio of nanotube that causes the enhancement of electric field close to the nanotube cap. In Fig. 1, calculated electric field lines and spatial distribution of electric field intensity near the nanotube's ends are presented for open and closed SWNTs. In these calculations, carbon nanotubes are considered to be metallic and Laplace's equation is solved numerically. In Fig. 1(b),(c) the color change represents the increase in the intensity of the electric field. We found that the field intensity in front of an open nanotube is higher than the field intensity in front of a closed nanotube. The field enhancement factor, β, is an important factor in field emission and it can be defined as $\beta = E_L/E_A$ where E_L is the local and E_A is the applied electric field. In our calculations, E_A is considered as the electric field very far away from the nanotube. Earlier, in order to estimate β of a protrusion, simple models were proposed [23] and numerical calculations were performed [23–25]. One of these is the 'hemisphere on a post' model and a simple expression in the form $\beta = m + h/\rho$ is used to express β where $m = 2$, h is the protrusion height and ρ is the hemisphere's radius [23,26]. Recent numerical calculations showed that this expression overestimated β, thus numerical calculations to estimate β are necessary [23–25].

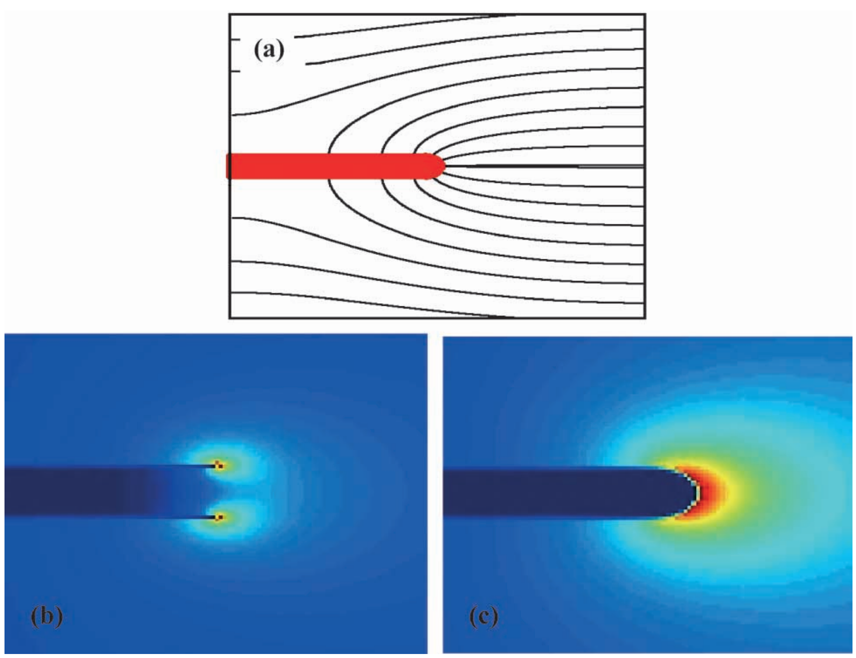

FIGURE 1 (a) Calculated electric field lines near a closed (5,5) nanotube's cap. (b) Spatial distribution electric field intensity near an open (5,5) tube's end. (c) near a closed (5,5) tube's cap. The color change from blue to yellow and to red represents increase in field intensity. (Colour version available online.)

Due to their higher field intensity very close to the nanotube's end, open nanotubes are expected to have higher β values. On the other side, β was found to depend on E_A and this field dependence of β and the spatial change in field intensity were found to be very important in the deviation of Fowler–Nordheim plots from straight lines [11]. Our numerical calculations presented here shows that the field intensity of open nanotubes decreases more rapidly with the distance from the end of the nanotube, which makes open nanotubes disadvantageous at low applied electric fields.

The current density from individual nanotubes is due to tunneling of electrons through a potential barrier. By incorporating the electrostatic potential and the effective potential of electrons from SCF-pseudopotential electronic structure calculations, the variation of potential energy of electrons and thus the potential barrier for tunneling are calculated. Furthermore, in order to understand the field emission mechanism and determine the dependence of emission current on important factors, current vs. applied field characteristics are calculated using the WKB approximation. The effective electronic potentials from SCF-pseudopotential calculations that contain the image potential and local density of electronic states from tight-binding calculations are also considered.

Recent experiments [27] and our recent investigations [11] have shown that longer nanotubes emit first and they have low turn-on and threshold field values. The deviation from linear Fowler–Nordheim behavior was found to be directly related to the variation of local electric field in the tunneling region [11]. The current vs. applied field calculations for closed (5,5) nanotubes in different heights are presented in Fig. 2.

In Fig. 3, Fowler–Nordheim plots are presented for open and closed nanotubes and for different nanotube sizes. The investigations presented here show that closed nanotubes emit more current then open nanotubes at low applied electric fields. However, this situation is reversed and open nanotubes emit more at higher applied electric fields. An important reason for this behavior is the variation of the electric field in the tunneling region. The electric field in the open tube case decreases faster with the distance; thus there is a relatively lower local electric field intensity further away from the nanotube end to reduce the tunneling barrier at low applied fields.

When the field enhancement and the electronic structure of nanotubes are considered, another important factor is appeared to be the nanotube diameter. The F–N plots of open (5,5) and (10,10) nanotubes are presented in Fig. 2(b). A (5,5) nanotube with relatively smaller diameter is found to have higher emission current.

The applied electric field values in these calculations are higher than the experimental values. On the other side, the field enhancement factor, β, increases linearly with nanotube length. Thus, in experiments, a long nanotube of 10 μm length has a high β value and needs only 1 V/μm as a turn-on field [27].

In field emission experiments employing nanotubes as electron emitters, field emission microscopy images are also observed. These images and their patterns are related with the local characteristics of the caps such as the presence of adsorbates on the caps [29]. Pentagonal regions were also observed in emission patterns that were related with the pentagonal rings in the caps [30]. In order to understand the form of the patterns and relate them to the local electronic structure of the cap, emission pattern simulations are performed. A screen is assumed which is 86 A away from the nanotube tip. Using the assumption that the electrons follow the electric field lines, the patterns they can form are calculated. In Fig. 3, the patterns

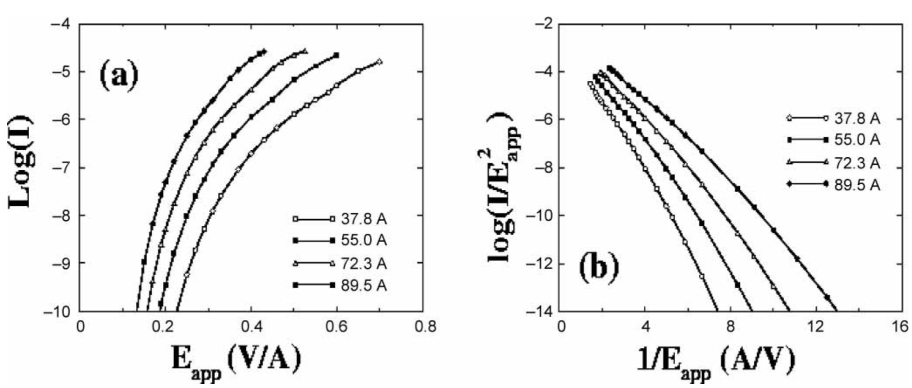

FIGURE 2 (a) Current vs. applied electric characteristics of field emission from closed (5,5) nanotubes of different heights. Hollow circles, filled squares, hollow triangles and filled circles are for nanotubes of 38, 55, 72 and 90 A, respectively. (b) Fowler–Nordheim plots of electron field emission from closed (5,5) nanotubes. A workfunction of 4.8 eV is considered [28].

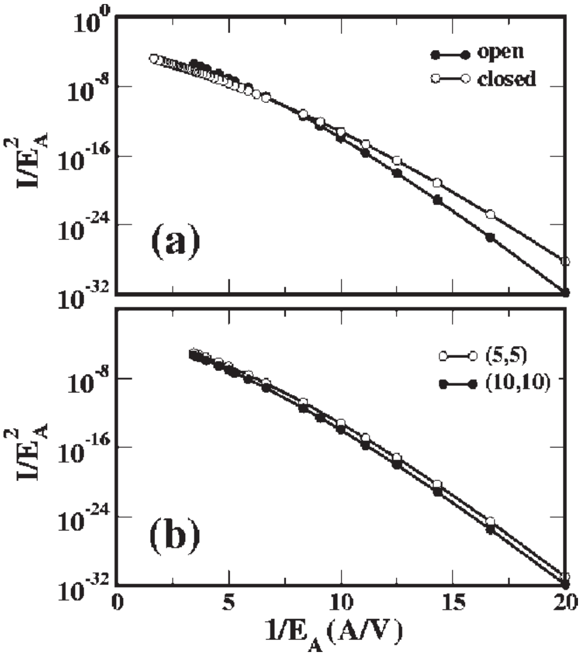

FIGURE 3 Fowler–Nordheim plots of electron field emission from open and closed nanotubes. (a) F–N plots of open and closed (10,10) tubes. Hollow circles are for the closed tube with 77 A length and dark circles are for the open tube with 68 A length. (a) F–N plots of open (5,5) and (10,10) tubes with the same lengths. Dark and hollow circles are for (10,10) and (5,5) tubes, respectively.

due to electron emission from a closed (10,10) nanotube are presented.

There is a pentagonal ring at the apex of a closed (10,10) nanotube and the atoms of the pentagonal ring are the first to start emitting electrons [11]. At low applied field only the atoms at the apex of the cap are emitting and the pattern shown in Fig. 4(a) is formed. By increasing the applied field, more atoms begin to emit. There are other five pentagonal rings in the cap and these have high local density of electronic states for field emission. In addition to these atoms, the other atoms bonded to these start to emit a significant amount of current at higher electric fields and the pattern presented in Fig. 4(b) is formed.

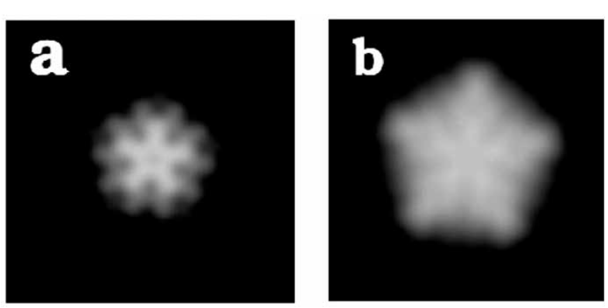

FIGURE 4 Simulated field emission patterns of a closed (10,10) nanotube (a) at a low applied electric field intensity (E_A = 0.18 V/A) and (b) at a high electric intensity (E_A = 0.40 V/A).

CONCLUSIONS

In conclusion, theoretical investigations on the field emission properties of open and closed single wall nanotubes are presented. The electric field is dramatically enhanced near the cap of a nanotube with a large variation of the local field distribution. It is found that the field intensity of an open nanotube in very close proximity of the tip is higher than the field intensity of a closed nanotube. On the other hand, the field intensity of open nanotubes decreases more rapidly with the distance to the end of the nanotube, which makes open nanotubes disadvantageous at low applied electric fields. The investigations presented here show that closed nanotubes emit more current than open nanotubes at low applied electric fields. However, the situation is reversed and open nanotubes emit more at higher applied electric fields. Emission patterns of closed nanotubes are found to be related to the local electronic structure at the nanotube cap.

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