Modelling of electron transfer from a carbon nanotube cap into the vacuum under high extraction fields

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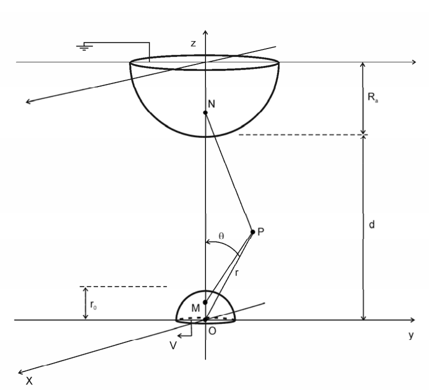
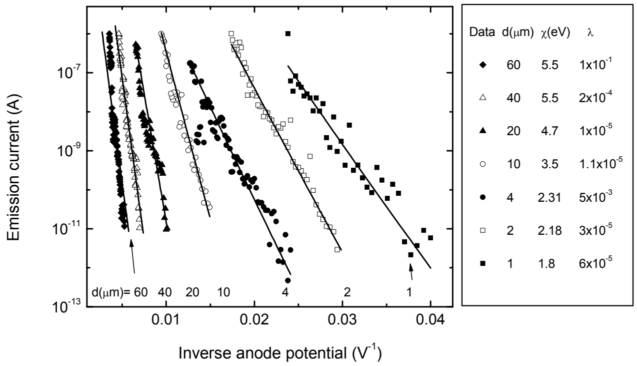


Figure 1

The Fowler-Nordheim (FN) theoretical model has been successfully used to explain the phenomenon of electron field emission (FE) from various metallic and semiconductor surfaces. One of the key parameters in the FN model is the local extraction field, which is usually very difficult to determine for real experimental setups. Consequently the field enhancement (i.e. the ration between the extraction and the macroscopic applied field) emerged as a necessary fitting parameter. The discovery of carbon nanotubes (CNTs) and other high aspect ratio structures introduced important supplementary difficulties when implementing the FN formalism. One such problem is the influence of the electronic structure on the FE process [1-4]. Other unique situations arise when the anode is moved very close to the emitter's tip, at distances comparable to its radius [5, 6] when structural changes to the potential energy barrier to the vacuum are likely to appear. In order to account for all these effects, a detailed model of the electron transfer from a CNT into the vacuum is needed.



Data	d(μm)	χ(eV)	λ
◆	60	5.5	1×10^{-1}
△	40	5.5	2×10^{-4}
▲	20	4.7	1×10^{-5}
○	10	3.5	1.1×10^{-5}
●	4	2.31	5×10^{-3}
□	2	2.18	3×10^{-5}
■	1	1.8	6×10^{-5}

Figure 2

In the present work, we consider a system of a grounded CNT of length L and radius r_0 (the *emitter*) facing a spherical anode of radius R_a ($R_a >> r_0$). The anode is placed at some distance away from the emitter's tip. The CNT is modelled as a two-dimensional (2D) manifold where electrons behave as quasi-free and independent particles [3, 4]. The electrons are bound on the CNT surface by a one-dimensional (1D) potential well, due to the restriction imposed by the cylindrical symmetry. The potential energy of the quasi-free electrons takes an overall position independent value of $-W_0$ (the origin of the energy scale is taken at the Fermi level). In order to have a full description of the electron behaviour in the

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whole system, a potential energy in the vacuum region needs also to be defined. To this purpose, the CNT cap is simplified as a grounded conducting sphere of radius r_0, facing the anode on the same symmetry axis (Fig. 1). As the emitter-anode distance, d and the anode radius, R_a are much greater than r_0, the electric field in vacuum may be computed using the method of electrostatic images. The electric potential follows then by integrating the field along convenient paths connecting the grounded cathode to any arbitrary point in space. The non-electrostatic energy jump, χ, at $r=r_0$ is taken into account as a separate parameter. Using this potential energy scheme, the solutions of the Schrödinger equation on the 2D CNT manifold [3, 4] are connected to the 3D ones in vacuum, which obey the radiating boundary condition. Having found the electronic wave function, the radial component of the probability current density in vacuum can be computed and from there the emission current follows allowing for a comparison to experimental current-voltage (I-V) diagrams. A set of data measured for several anode-to-cathode separations was used in the present analysis. The first approach was to keep a fixed vacuum barrier height and fit the experimental data with the enhancement factor only. As no consistent results have been obtained a second approach was tried: allowing the vacuum barrier height to vary with the anode-to-cathode separation as a fitting parameter in the aforementioned electrostatic model. The fitting results are presented in Fig. 2. The best fit values of the barrier height for different anode-to-cathode separations are presented in Fig. 3. It may be concluded that when the anode gets closer to the emitter its electronic behaviour is perturbed and the barrier height tends to decrease. This may be an effect of local transitory ionizations of atoms at the CNT tip. Obviously, the change in the local field enhancement may also play an important role in this phenomenon, but the purpose of the present analysis is to emphasize the possibility of variation of the barrier height in such circumstances, an aspect which is usually overlooked in current FN approaches.

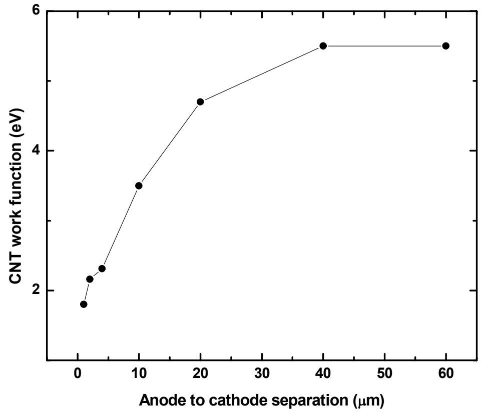

Figure 3

References

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