Field enhancement properties of nanotubes in a field emission set-up

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Controversy in the mechanisms of emission

Modeling of the polarization of CNT

- Resolution of the Poisson's equation
- Use of an atomic dipolar approximation
- The local field is computed with the Lippmann-Schwinger's equation

$\beta$ factor for SWNT:

- evolution with the length
- evolution with the diameter
- influence of the density

$\beta$ factor for MWNT

Thanks and conclusions
Flat panel displays:
- Low turn-on field
- Low sensitivity to the vacuum conditions
- High Brightness

NEA materials:
Diamond type films:
- Emission from localized sites
- Emission mechanisms not well known

Ultra Thin SC film:
- Emission properties due to nanometer thickness
- Uniform emission
- Mechanism: Electronic injection → bending of the conduction band

Carbone nanotubes:
- $v_{\text{turn-on}} \leq 1 \text{ V/μm}$
- Prototype of display already achieved

Nanotubes forest:


Multi-wall Nanotubes:


Mechanisms of emission

The mechanism leading to the electronic emission at low field is not well understood

⇒ Several phenomena are suspected to be involved

- Enhancement of the applied field:
  - Polarization phenomenon
  - Localized space charge
- Implication of localized states at the end of the nanotubes
- Uniform and atomic descriptions lead to contradictory results
- Is Fowler-Nordheim still valid?

Energy Distributions

\[ E = 0.15 \text{ V/Å} \quad E = 0.20 \text{ V/Å} \quad E = 0.30 \text{ V/Å} \]

\[ I_M = 3 \times 10^{-10} \text{ nA} \quad I_M = 5 \times 10^{-4} \text{ nA} \quad I_M = 100 \text{ nA} \]

\[ E = 0.15 \text{ V/Å} \quad E = 0.20 \text{ V/Å} \quad E = 0.30 \text{ V/Å} \]

\[ I_M = 3 \times 10^{-9} \text{ nA} \quad I_M = 2 \times 10^{-3} \text{ nA} \quad I_M = 10^5 \text{ nA} \]
Theoretical background

◊ Aim: Compute electrostatic field near nanotube's end
◊ Model: Atomic dipoles and perfect metal

⇒ Self-consistent resolution of Maxwell-Gauss's law:

\[ \vec{\nabla}_r \cdot \vec{E}(\vec{r}) = -\frac{1}{\varepsilon_0} \vec{\nabla} \cdot \vec{P} = \vec{\nabla}_r \cdot \left[ \sum_{j=1}^{N_{at}} \vec{\alpha}_j \delta(\vec{r} - \vec{r}_j) \vec{E}(\vec{r}_j) \right] \]

⇒ \( \vec{E}(\vec{r}) \) solution of the Lippmann-Schwinger's equation:

\[ \vec{E}(\vec{r}) = \vec{E}_0(\vec{r}) + \sum_{j=1}^{N_{at}} \vec{S}_0(\vec{r}, \vec{r}_j) \cdot \vec{\alpha}_j \cdot \vec{E}(\vec{r}_j) \]

◊ Local field → \( \beta = \frac{E_{loc}}{E_{app}} = \frac{Max(E_z)}{E_0} \)

Polarization potential

(5,5) capped nanotube
Single wall nanotubes

general trend: 
\[ \beta(L) = L \times [a_0 + a_1 \ln(L) + a_2 \ln^2(L) + \ldots] \]

- Saturation of the \( \beta \) factor with the length
- Saturation sets up faster for \((n,n)\)
- The caps improve the \( \beta \) factor but do not modify the general trend
- No significant influence of the chiral angle
- Extrapolation for a length of 1 \( \mu \text{m} \): \((6,0)\) capped \(\rightarrow\) \( \beta \simeq 1100 \)
Variation with the diameter

\[ L = 30 \text{ nm} \quad \text{and} \quad L = 1 \mu\text{m} \text{ (extrapolated)} \]

\( (n,0) \) nanotubes

\[ \beta(D) = a_0 + \frac{a_1}{D} + \frac{a_2}{D^2} + \frac{a_3}{D^3} + \ldots \]

\( \beta \geq 1000 \) can only be obtained with \( D \leq 0.5 \text{ nm} \)

\( \beta \) for a \((9,0)\), \( \beta \) is only around 200

\( \Rightarrow \) Phenomena other than polarization are probably involved in the emission
Influence of the density

Polarization potential in the $XY$ plane (top) at $Z = 8.5$ nm and $XZ$ plane (bottom) at $Y = 0$ for a rope of 13 (6,0) nanotubes

- The $\beta$ factor decreases when the density is increased
- To have a uniform emission $\rightarrow$ decrease the density
- The polarization is larger for the external nanotubes
- The $X$ $Y$ components of the field are larger than the $Z$ component
- Emission from the brim of the rope $\rightarrow$ large opening of the beam
Multi wall nanotubes

(3,3)@(13,5) and (3,3)@(15,2)  (9,0)@(19,1) and (9,0)@(15,7)

- No significant influence of chirality
- The maximum value of the $\beta$ factor is given by the inner shell
- The addition of shells tends to sweep out the instabilities of the $\beta$ factor
- The outer shells tend to reduce the enhancement property of the inner shell $\rightarrow$ Faraday cages
Conclusions

⇒ No influence of the band structure on the polarization

⇒ Saturation of the polarization with the length of the nanotubes

⇒ The saturation sets up faster for (n,n) nanotubes

⇒ (n,0) nanotubes are the best field amplifier

⇒ The largest $\beta$ factor observed for isolated SWNT is only of the order of 200 → other phenomena are probably involved

⇒ In the case of a rope, the induced field is larger close to the brim

⇒ The field amplification of MWNT seems to be due to small inner tubes

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