

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

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Framework

- ◇ 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
- ◇ β factor for SWNT:
 - evolution with the length
 - evolution with the diameter
 - influence of the density
- ◇ β factor for MWNT
- ◇ Thanks and conclusions

◇ Flat panel displays:

- Low turn-on field
- Low sensitivity to the vacuum conditions
- High Brightness

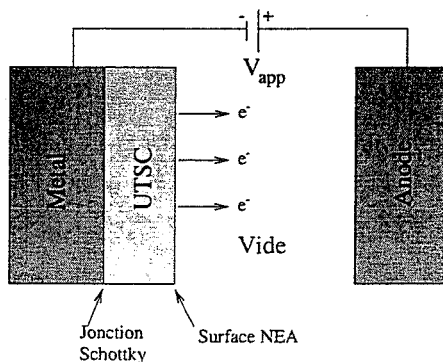
NEA materials:

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



Vu Thien Binh, Adessi, PRL 85 (2000)

Carbone nanotubes:

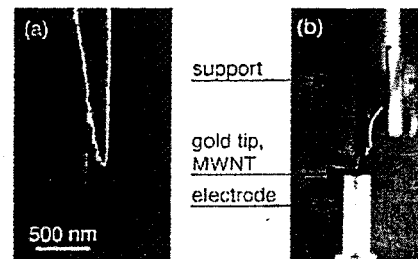
- turn-on field $\leq 1 \text{ V}/\mu\text{m}$
- Prototype of display already achieved

Nanotubes forest:



Z. F. Ren, Science 282 (1998)

Multi-wall Nanotubes:



J.-M. Bonard, Appl. Phys. A 69 (1999)

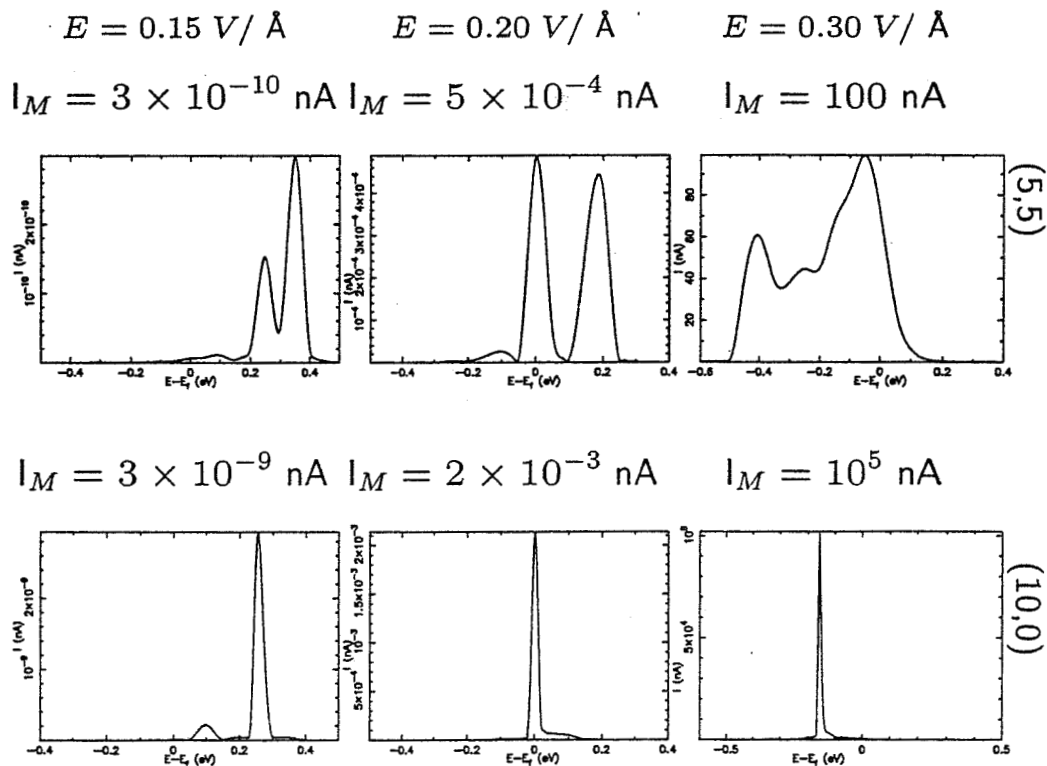
Mechanisms of emission

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



Theoretical background

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

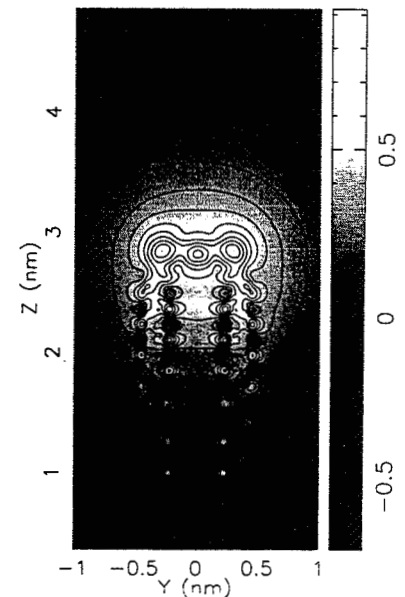
⇒ Self-consistent resolution of Maxwell-Gauss's law:

$$\vec{\nabla}_{\vec{r}} \cdot \vec{E}(\vec{r}) = -\frac{1}{\epsilon_0} \vec{\nabla} \cdot \vec{P} = \vec{\nabla}_{\vec{r}} \cdot \left[\sum_{j=1}^{N_{at}} \vec{\alpha}_j \delta(\vec{r} - \vec{r}_j) \vec{E}(\vec{r}) \right]$$

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

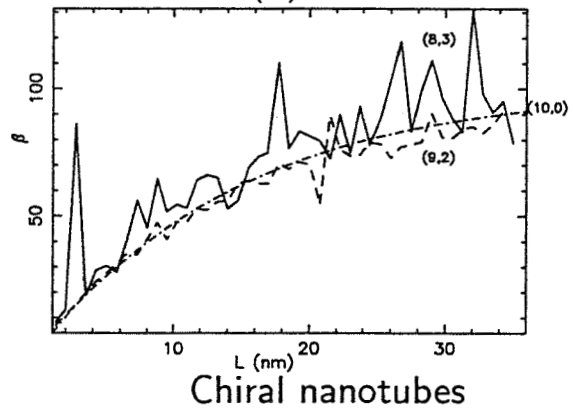
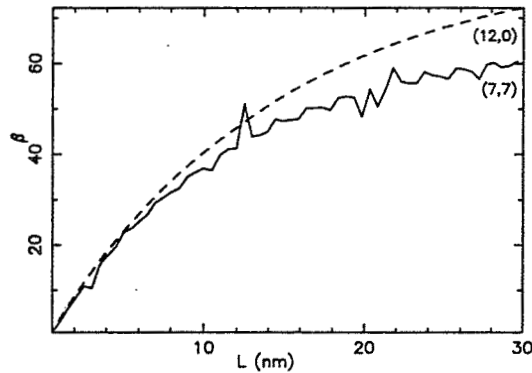
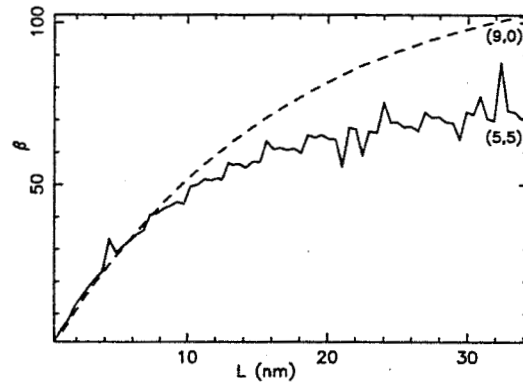
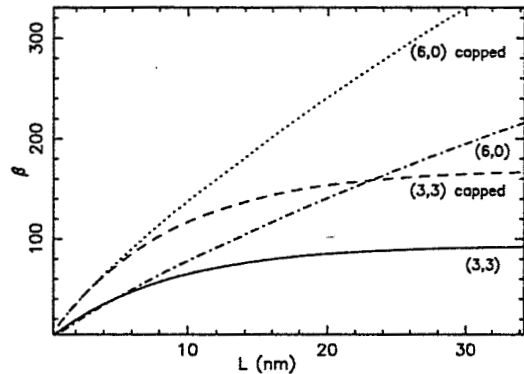
$$\vec{E}(\vec{r}) = \vec{E}_0(\vec{r}) + \sum_{j=1}^{N_{at}} \vec{S}_0(\vec{r}, \vec{r}_j) \cdot \vec{\alpha}_j \cdot \vec{E}(\vec{r}_j)$$

- ◇ Local field $\rightarrow \beta = \frac{E_{loc}}{E_{app}} = \frac{Max(E_z)}{E_0}$



*Polarization potential
(5,5) capped nanotube*

Single wall nanotubes



Chiral nanotubes

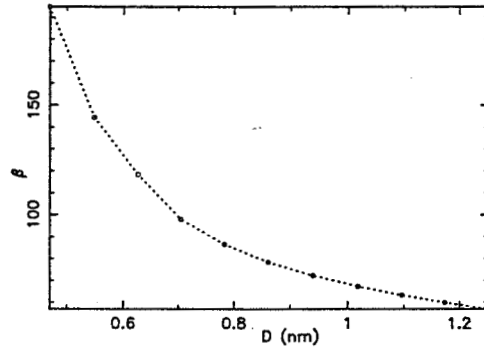
general trend:

$$\beta(L) = L \times [a_0 + a_1 \ln(L) + a_2 \ln^2(L) + \dots]$$

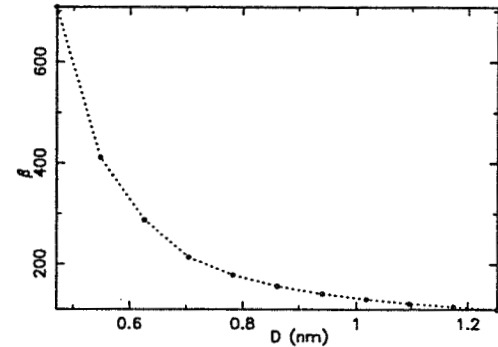
- ◇ Saturation of the β factor with the length
- ◇ Saturation sets up faster for (n,n)
- ◇ The caps improve the β factor but do not modify the general trend
- ◇ No significant influence of the chiral angle
- ◇ Extrapolation for a length of 1 μm : (6,0) capped $\rightarrow \beta \simeq 1100$

Variation with the diameter

$L = 30 \text{ nm}$



$L = 1 \mu\text{m}$ (extrapolated)



(n,0) nanotubes



(6,0)

$D = 0.47 \text{ nm}$



(11,0)

$D = 0.86 \text{ nm}$



(16,0)

$D = 1.25 \text{ nm}$

◇ Variation law:

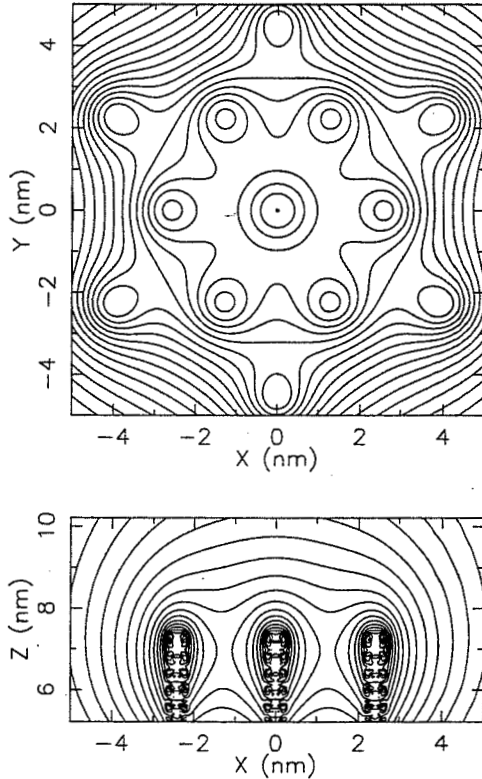
$$\beta(D) = a_0 + \frac{a_1}{D} + \frac{a_2}{D^2} + \frac{a_3}{D^3} + \dots$$

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

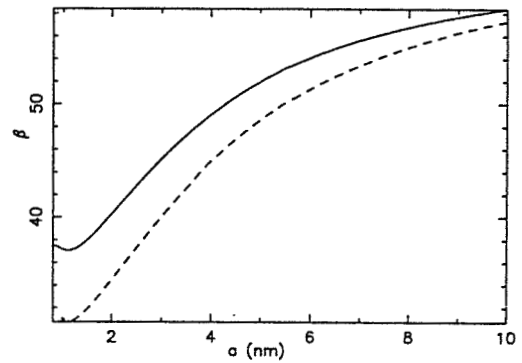
◇ For a (9,0), β is only around 200

⇒ 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

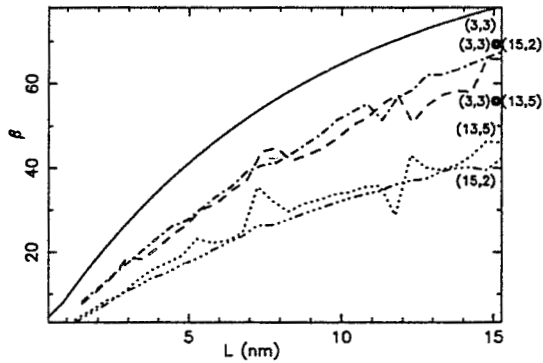


Evolution of the β factor with the mesh parameter. Solid line \rightarrow first nearest neighbors, dashed line \rightarrow first+second nearest neighbors

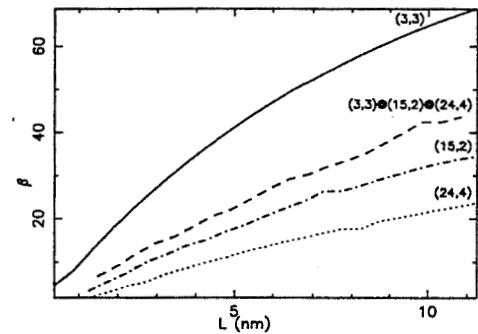
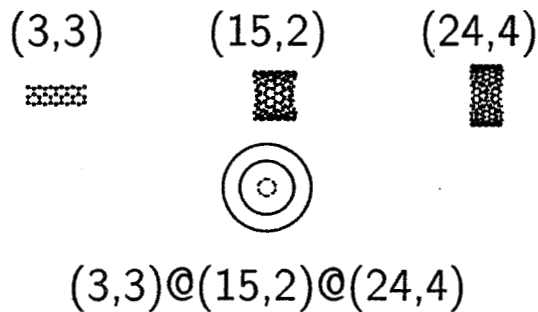
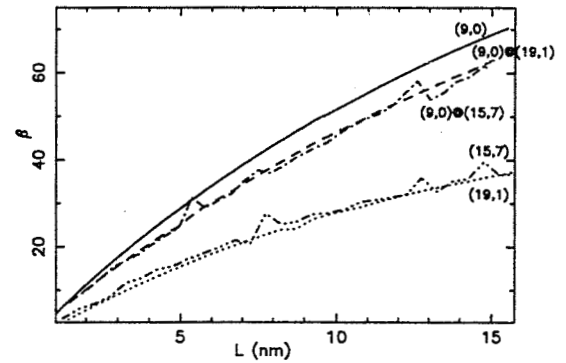
- ◇ The β factor decreases when the density is increased
- \Rightarrow To have a uniform emission \rightarrow decrease the density
- ◇ The polarization is larger for the external nanotubes
- ◇ The X Y components of the field are larger than the Z component
- \Rightarrow Emission from the brim of the 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 β factor is given by the inner shell
- ◇ The addition of shells tends to sweep out the instabilities of the β 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 β 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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