



SMR/1758-2

"Workshop on Ion Beam Studies of Nanomaterials:  
Synthesis, Modification and Characterization"

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**Ion Channeling through Carbon Nanotubes**

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# Ion channeling through carbon nanotubes

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S. Petrovic  
D. Borka

*Support:* NSERC & PREA



# Outline

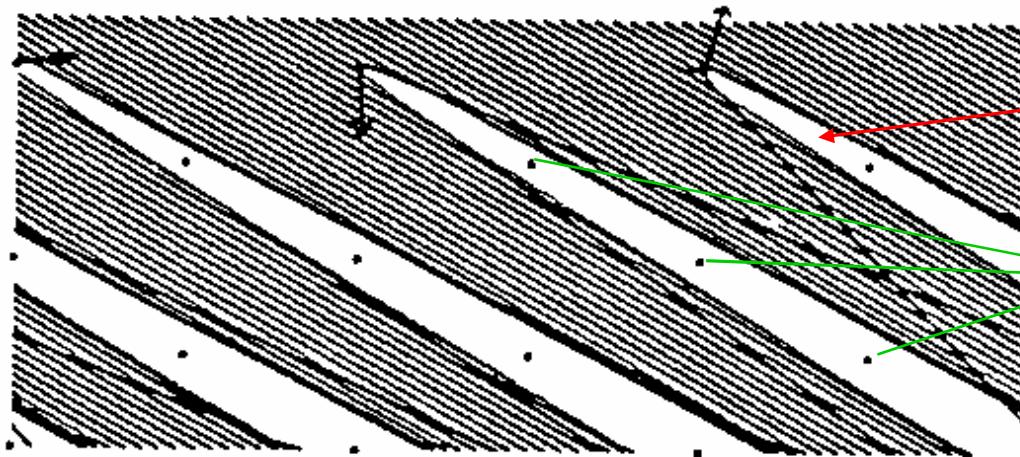
- **Reminder: Channeling in single crystals**
- **Ion interactions with carbon nanotubes**
- **High-energy channeling (~GeV)**
  - Potentials and beam deflection
  - Rainbow effect in short ropes
- **Medium-energy channeling (~MeV)**
  - Modeling the dynamic response
  - Simulations of ion distributions
  - New developments
- **Low-energy channeling (~keV)**
  - MD simulations
  - Related problems
- **Outlook**

# Ion channeling in crystals

- “Accidental” discovery in computer simulation  
(1963)
- Theory:
  - Continuum-potential models
  - Binary collision approximation
  - De-channeling, ...
- Applications:
  - Medium energies:
    - ion implantation
    - probing impurities in crystals
    - thin films & interface analysis
  - High-energy physics:
    - using bent crystals for beam extraction & collimation at particle accelerators (CERN, JINR, FNAL, BNAL, IHEP, INFN-LNF)

# Channeling of fast ions in single crystals

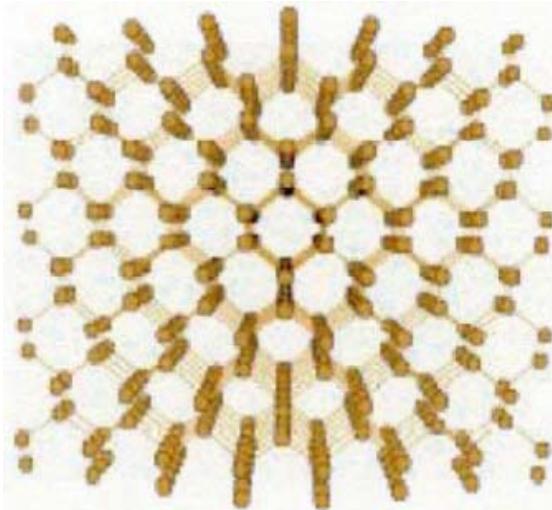
Side view of ion beam channeling



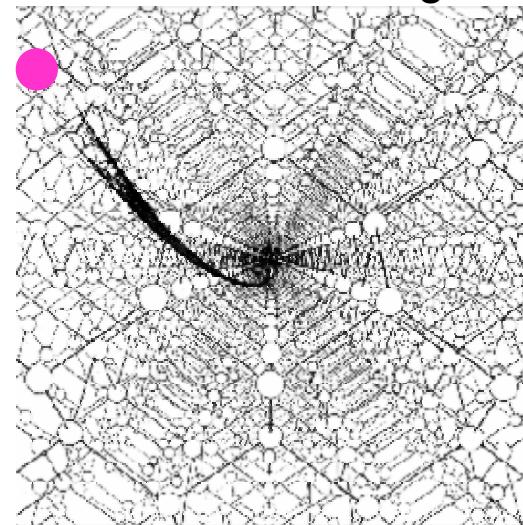
Shadow cone

Average potential  
along atomic rows

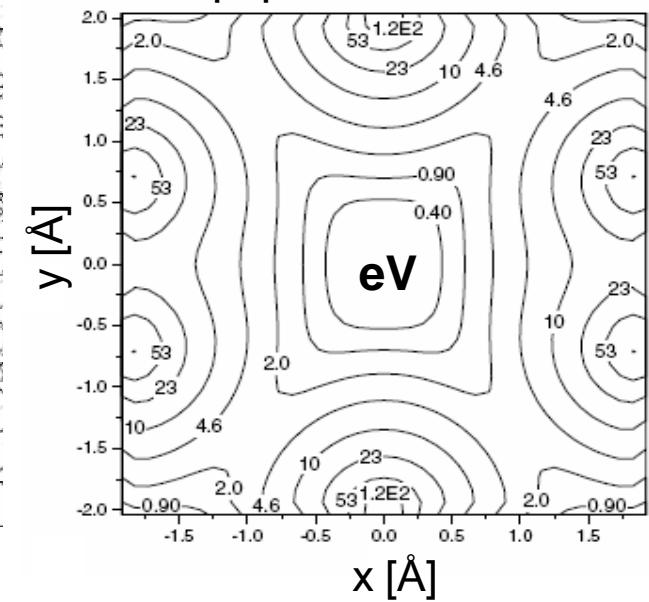
Front view of Si channels



Axial channeling



Equipotential curves

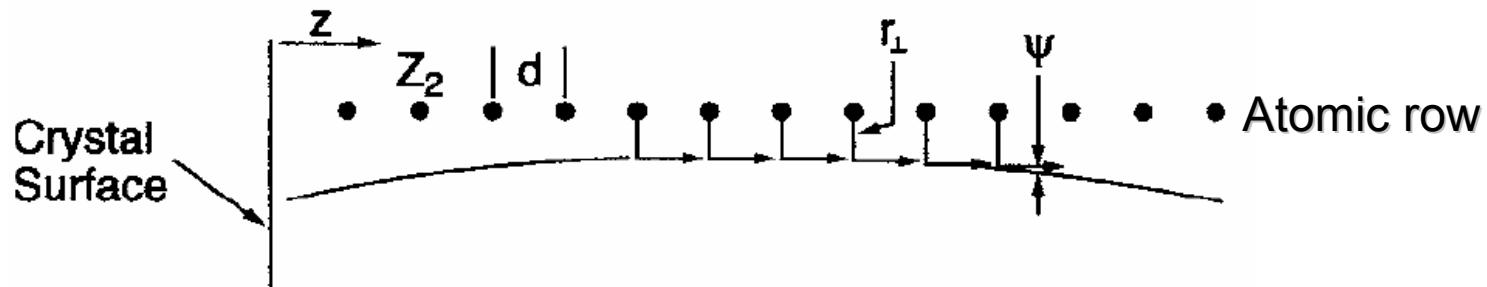


# Axial channeling through single crystal

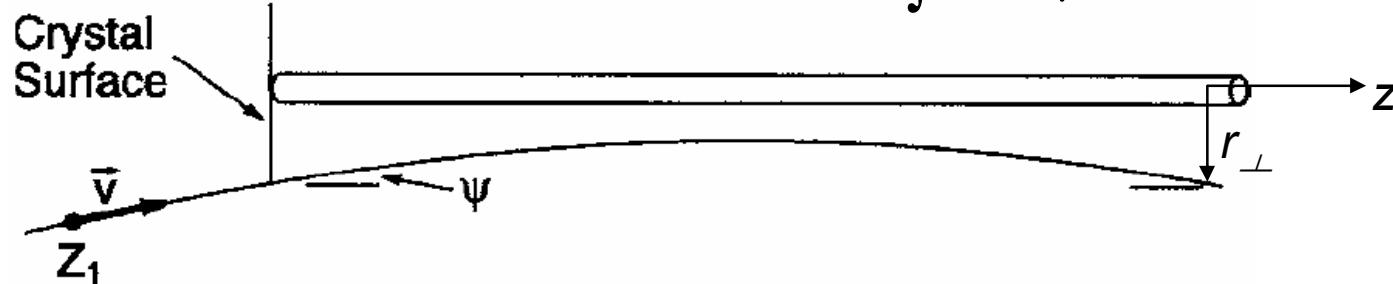
L.C. Feldman et al., *Materials Analysis by Ion Channeling* (1982)

## BINARY COLLISION MODEL

U.I. Uggerhoj



## CONTINUUM MODEL



Ion trajectory in transversal plane  $E_{\perp} = \frac{p^2}{2} \psi^2 + U_{row}(r_{\perp}) + \frac{L_0^2}{2m\gamma r_{\perp}^2} = const$

Critical angle for channeling

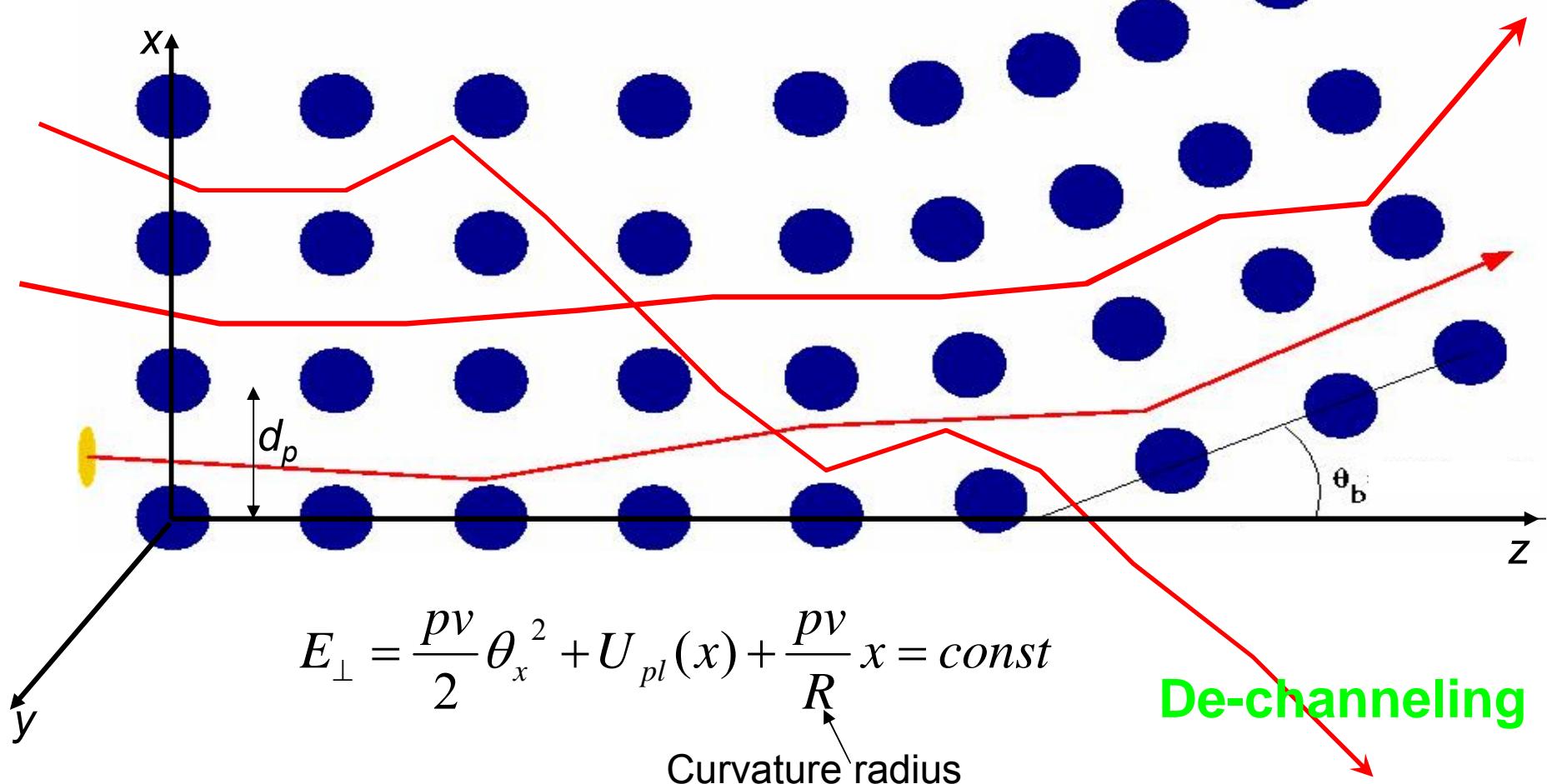
$$\psi_c = \sqrt{\frac{4Z_1 Z_2 e^2}{pvd}}$$

# Planar channeling through crystal bent in x direction

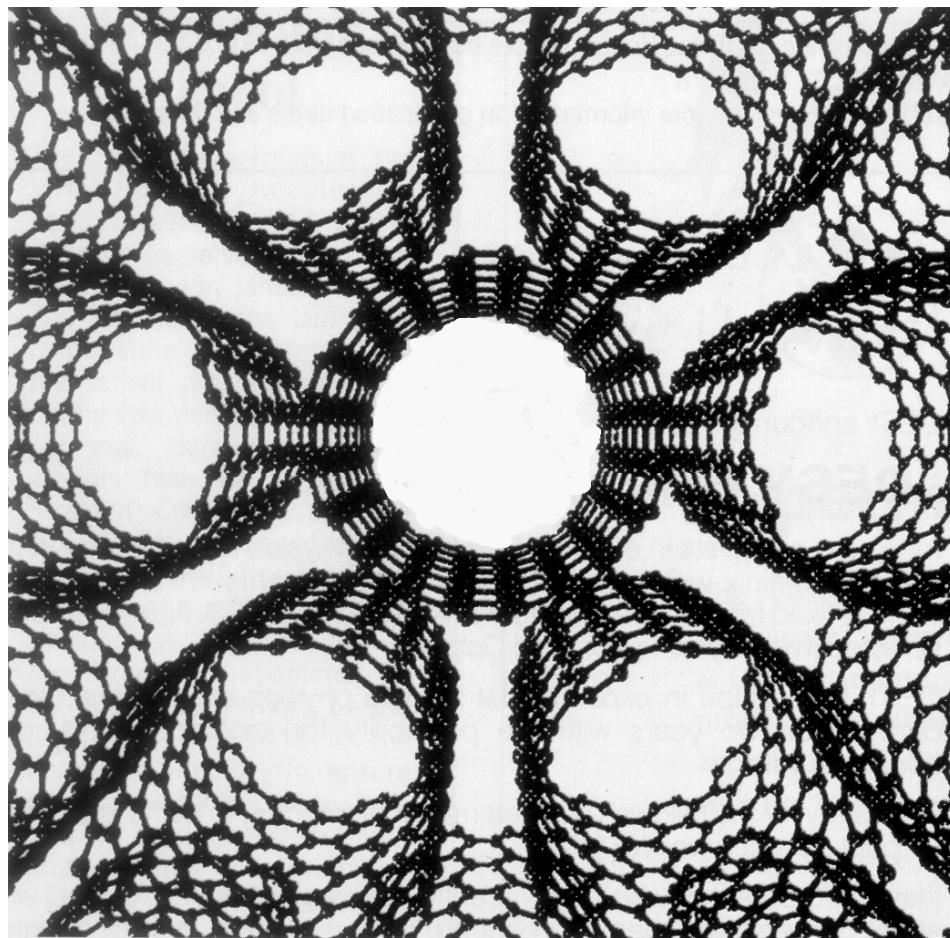
V.M. Biryukov et al., *Crystal Channeling and Its Applications at High-energy Accelerators* (1997)

R. Fliller III

Potential of single plane  $U_{pl}(x) = N_{at} d_p \int U_{at}(\sqrt{x^2 + y^2 + z^2}) dy dz$



# Ion channeling through carbon nanotubes? Dream vs. reality



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# Carbon nanotubes

## ❑ Properties:

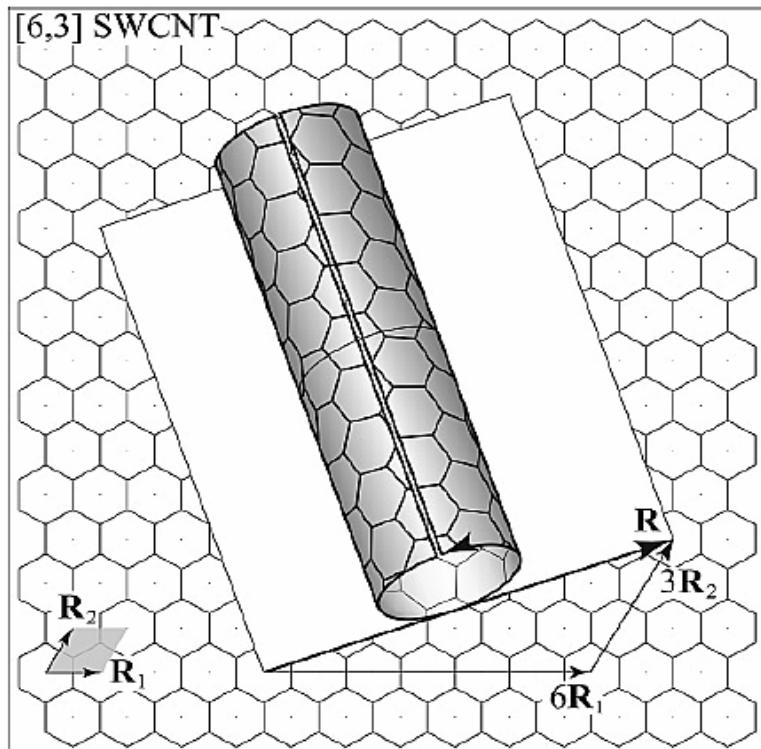
- Electrical, mechanical, thermal
- Dependent on: molecular structure, geometric confinement, local modification

## ❑ Applications:

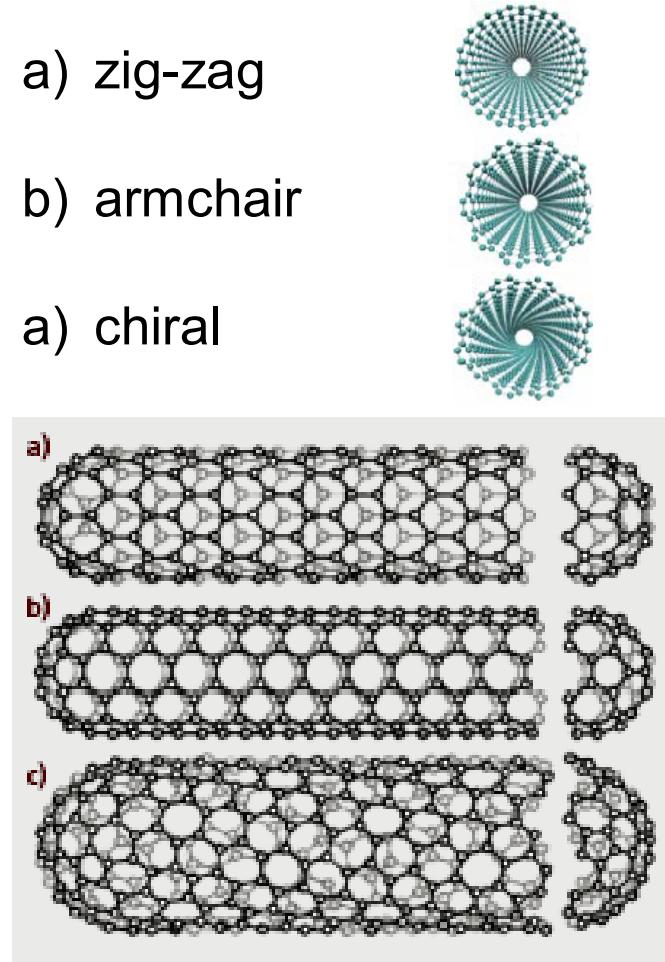
- Nanoelectronic devices
- New composite materials
- Sensitive chemical detectors
- Ion storage (H, Li)
- Field emission displays
- Nanoelectromechanical systems (NEMS)

# Formation of single-wall carbon nanotube (SWNT)

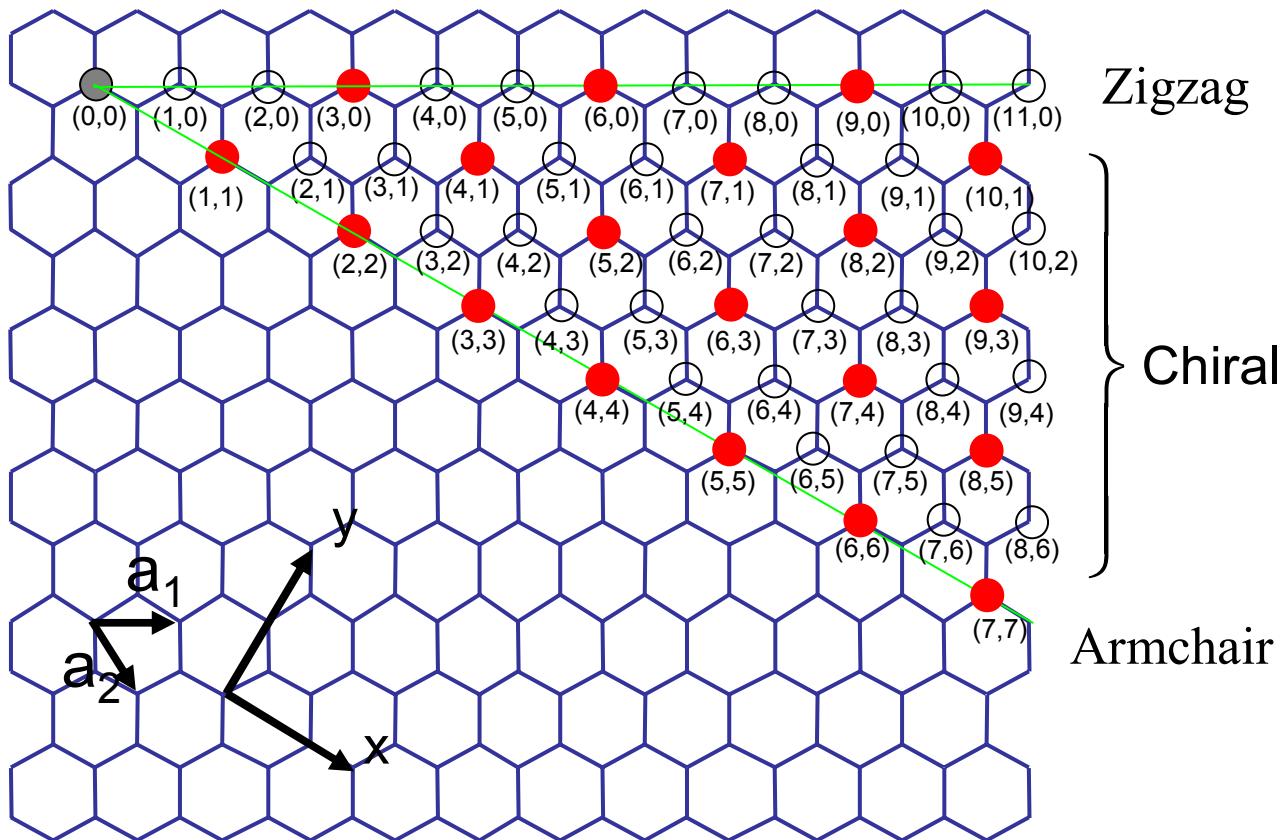
Rolling single graphene sheet:  
hexagonal lattice ( $d=0.14$  nm)  
of covalently bonded C atoms



Diameter  $\sim 1 - 2$  nm, Length  $\sim 1$  mm



# (n,m) nomenclature of SWNTs

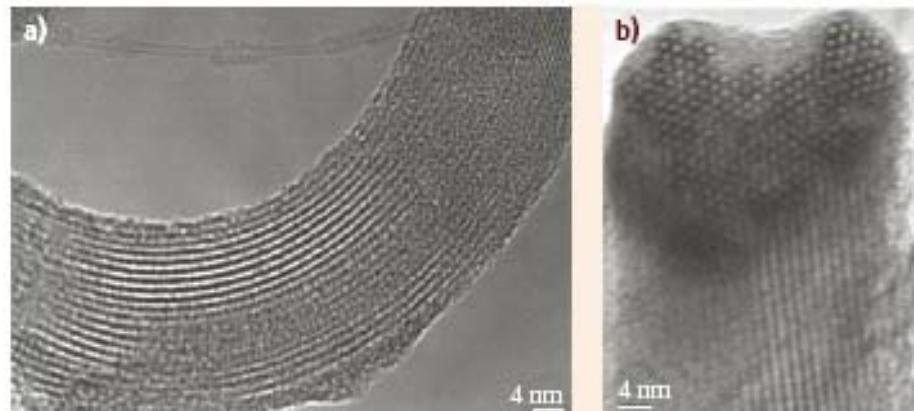


$n - m = 3q$  ( $q$ : integer): metallic

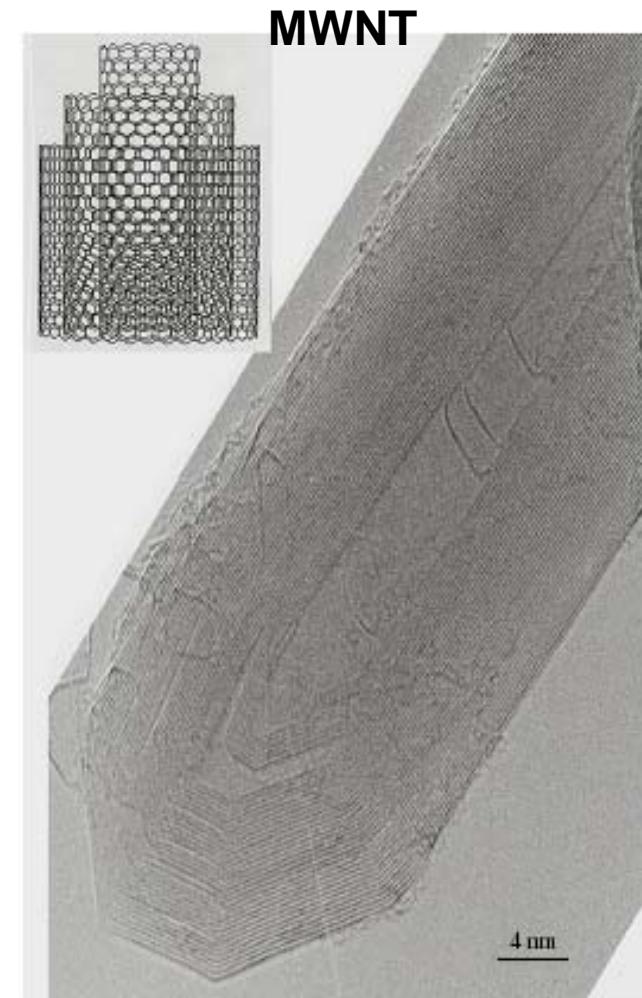
$n - m \neq 3q$  ( $q$ : integer): semiconductor

# Stacking of nanotubes by van der Waals forces with inter-wall separations $\sim 0.34$ nm

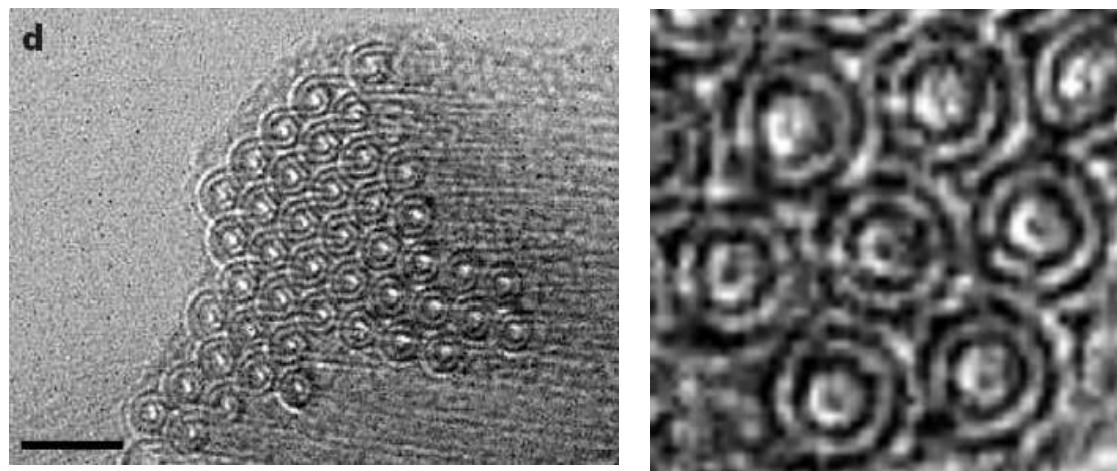
Rope of SWNTs in hexagonal lattice



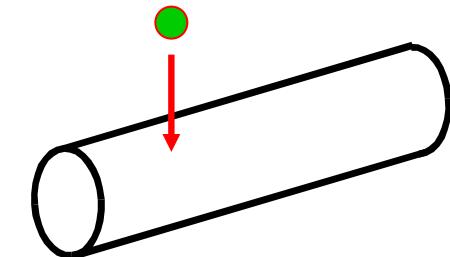
Multi-walled carbon nanotube



Rope of DWNTs in hexagonal lattice



# Ion irradiation of carbon nanotubes



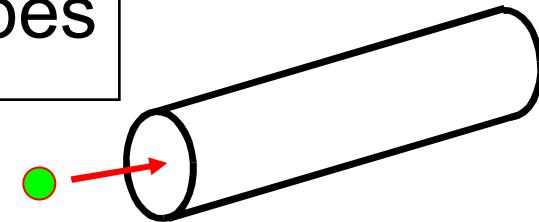
## □ Beam characteristics:

- Directions oblique or perpendicular to nanotube
- Energies from  $\sim 100$  eV to  $\sim 100$  MeV
- Heavy and light ions
- Strong dependence on irradiation dose
- Beam diameter for local modifications (FIB)

## □ Effects on nanotubes:

- Creation of local defects ( $\sim 20$  eV per atom)
- Doping, functionalization
- Inter-tube junctions (with high-T annealing)
- Amorphization, welding
- Stiffening, bending, buckling
- Observed by: SEM, TEM, RS, FEM, AFM, STM, ...

# Ion channeling through carbon nanotubes



## □ Advantages over single crystals

- Wider channels: weaker dechannelling
- Broader beams (using nanotube ropes)
- Wider acceptance angles ( $\sim 0.1$  rad)
- Lower minimum ion energies (< 100 eV)
- 3-D control of beam bending over greater lengths

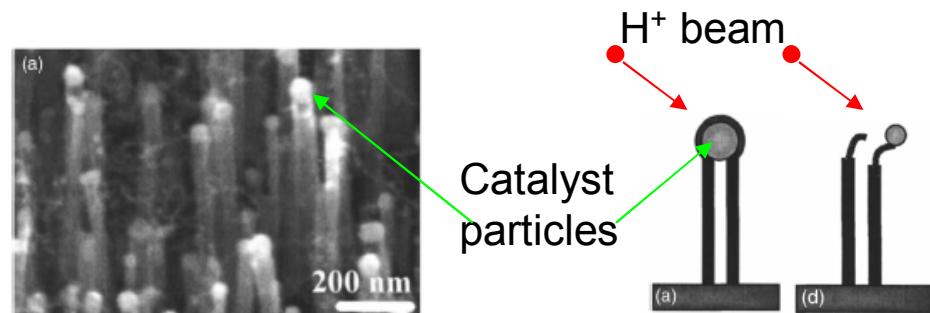
## □ Applications

- Creating and transporting highly focused nano-beams
- Nano-implantation in electronics, biology & medicine
- Beam extraction, steering & collimation at accelerators
- Manipulate plasma deposition, molecule transmission
- Sources of hard X- and gamma-rays

# Some issues regarding realization of channeling

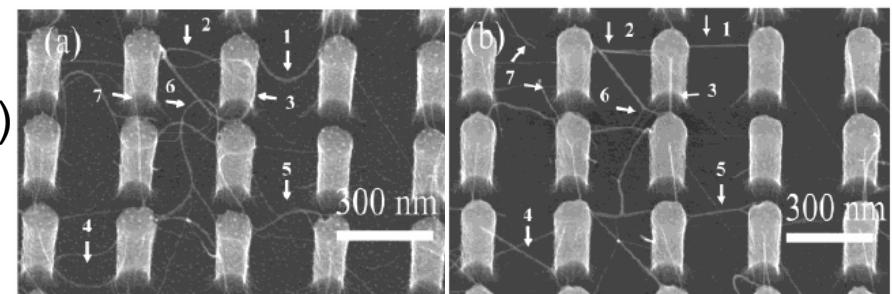
## □ Open ends (sputter etching)

J.F. AuBuchon *et al.*,  
*J. Appl. Phys.* 97 (2005) 124310



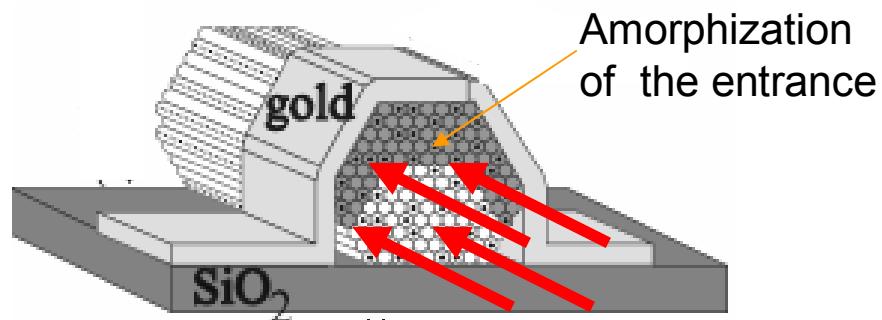
## □ Straightening (using Ga<sup>+</sup> beam)

Y.J. Jung *et al.*,  
*Nano Letters* 4 (2004) 1109



## □ Clamping by metal wires

H. Stahl *et al.*,  
*Phys. Rev. Lett.* 85 (2000) 5186



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# Continuum approximation for nanotube wall potential

- Repulsive potential of a C atom,  $U_{at}(R)$  (Lindhard, Molière, Doyle-Turner)
- Atomic row potential from longitudinal average

$$U_{row}(r) = \frac{1}{d_{at}} \int_{-\infty}^{\infty} U_{at}(\sqrt{r^2 + z^2}) dz$$

- Wall potential for zig-zag and armchair nanotubes with radius  $|r_j| = a$

$$U_{z,a}(r, \varphi) = \sum_{j=1}^N U_{row} \left( \sqrt{r^2 + a^2 - 2ra \cos(\varphi - \varphi_j)} \right)$$

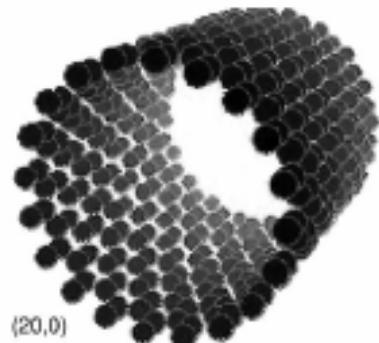
- Wall potential for chiral nanotubes with radius  $a$  from averaging over circumference

$$U_{chi}(r) = a\sigma_{at} \int_0^{2\pi} \int_{-\infty}^{\infty} U_{at} \left( \sqrt{z^2 + r^2 + a^2 - 2ra \cos \varphi} \right) dz d\varphi$$

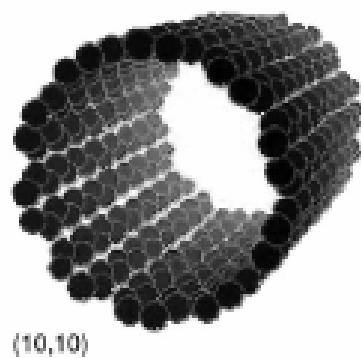
# Continuum approximations for the repulsive atomic potential in SWNTs

X. Artru *et al.*, *Phys. Reports* 412 (2005) 89

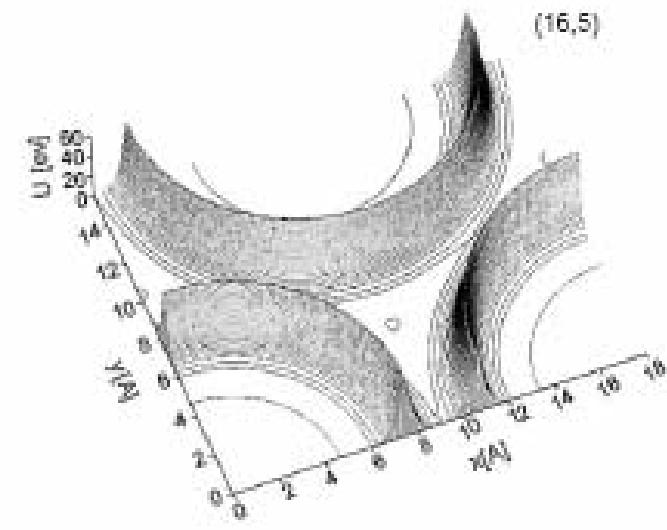
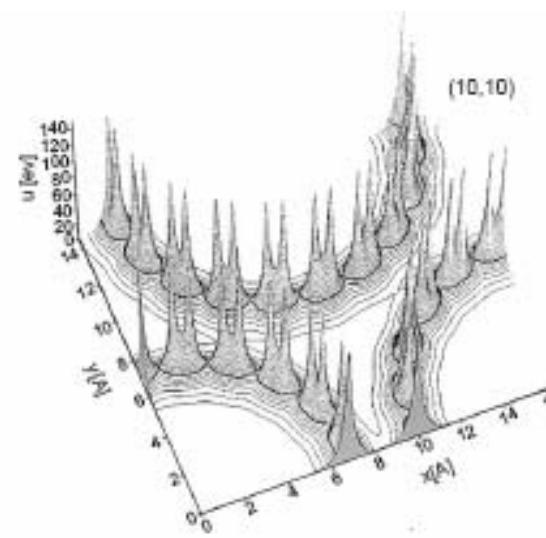
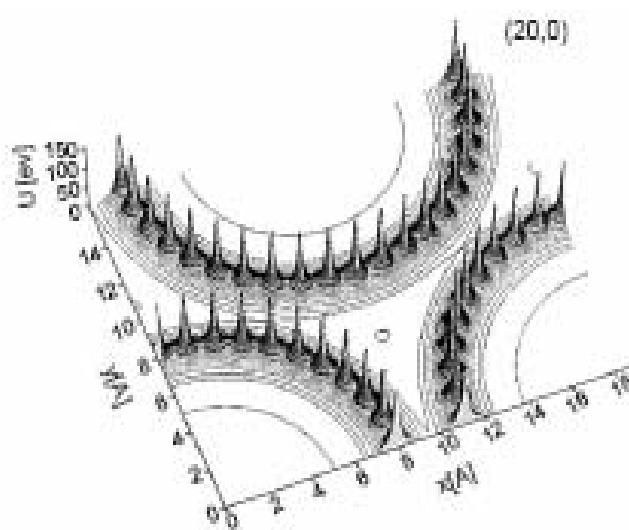
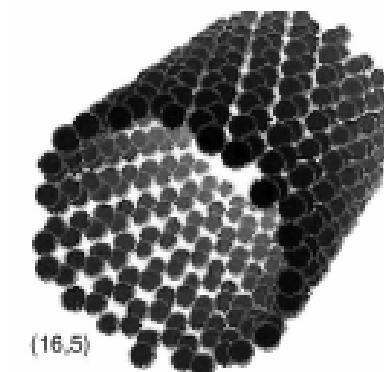
Zig-zag



Armchair

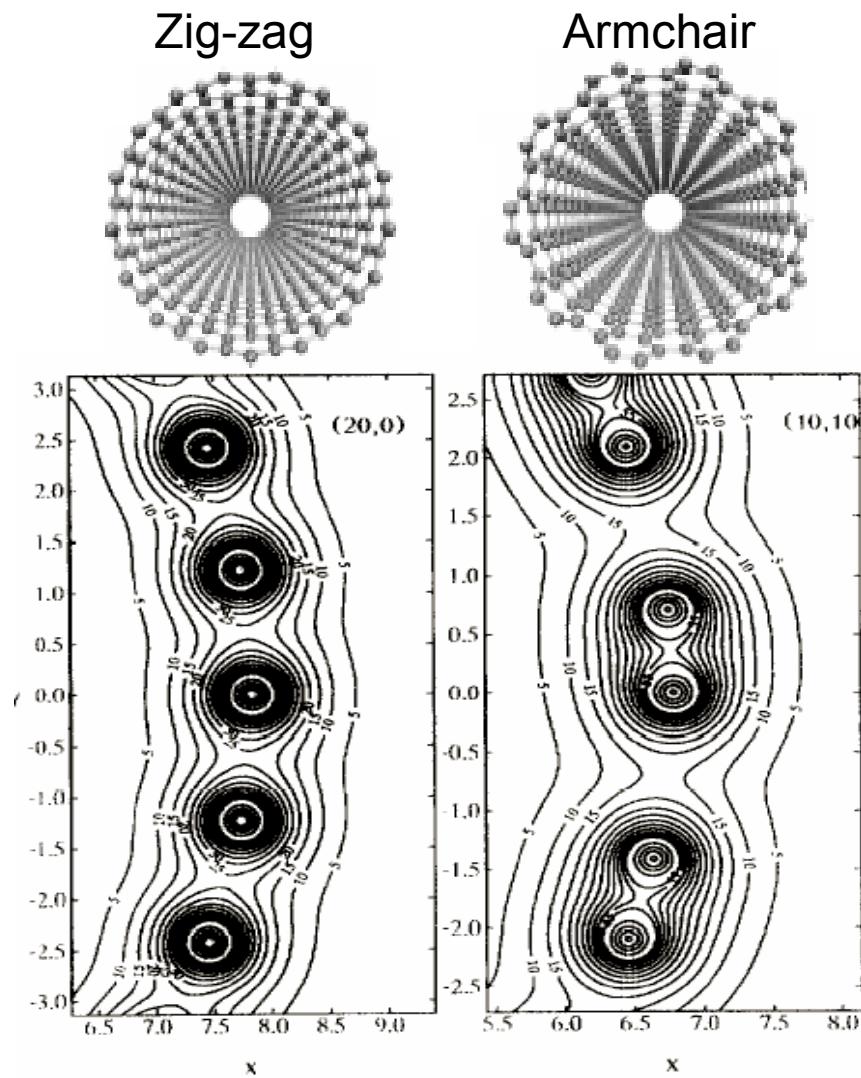


Chiral

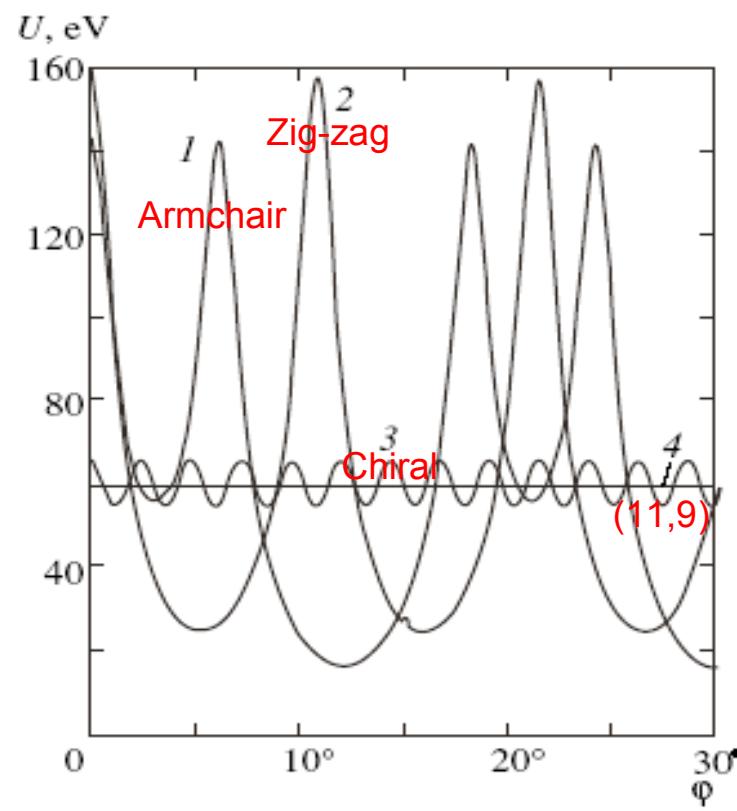


# Continuum potential due to atomic rows in achiral SWNTs

N.K. Zhevago and V.I. Glebov, *J.E.T.P.* 91 (2000) 579

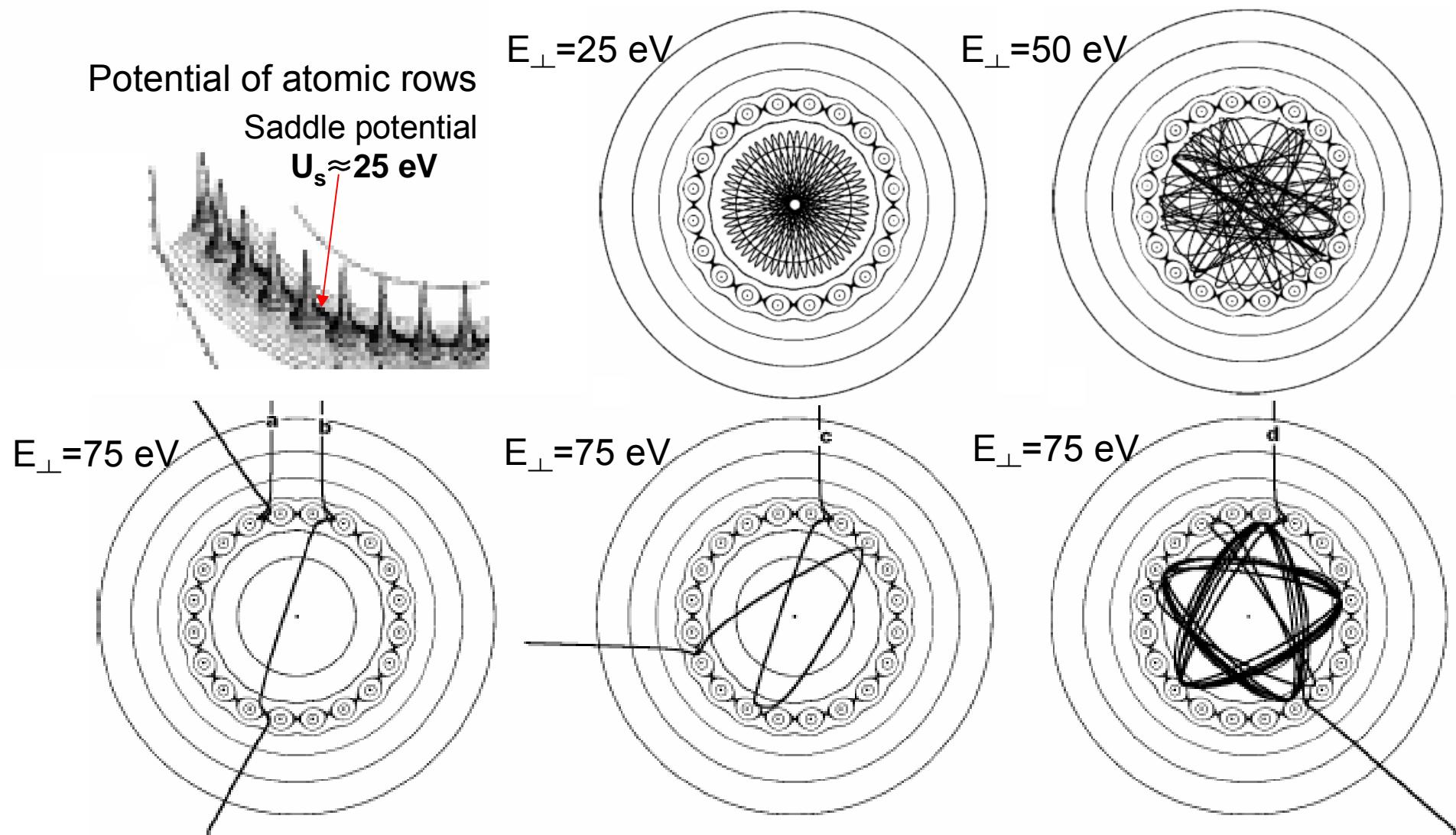


Angular variation of potential barrier at the nanotube wall



# Trajectories for ion channeling in a zig-zag SWNT<sub>(10,0)</sub> at several transverse energies $E_{\perp}$ relative to saddle $U_s$

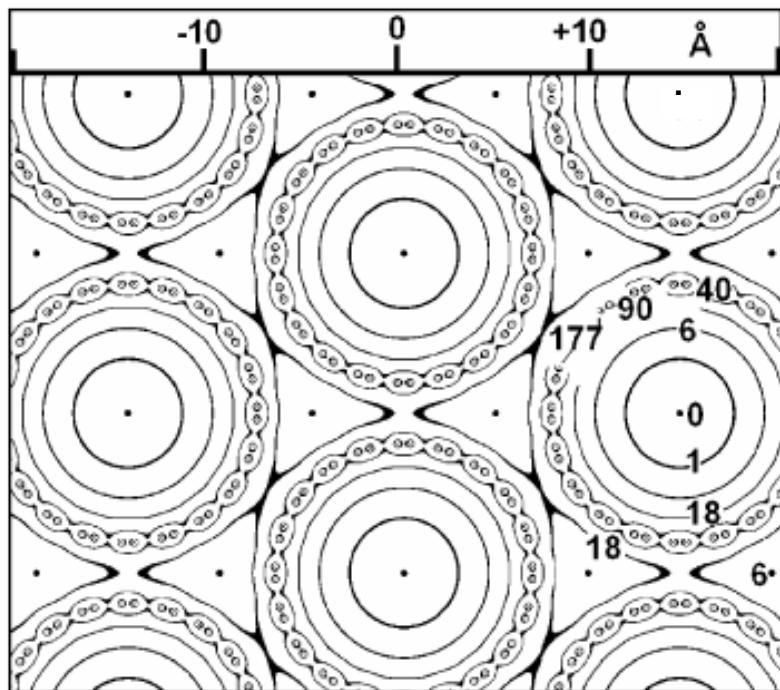
X. Artru *et al.*, *Phys. Reports* 412 (2005) 89



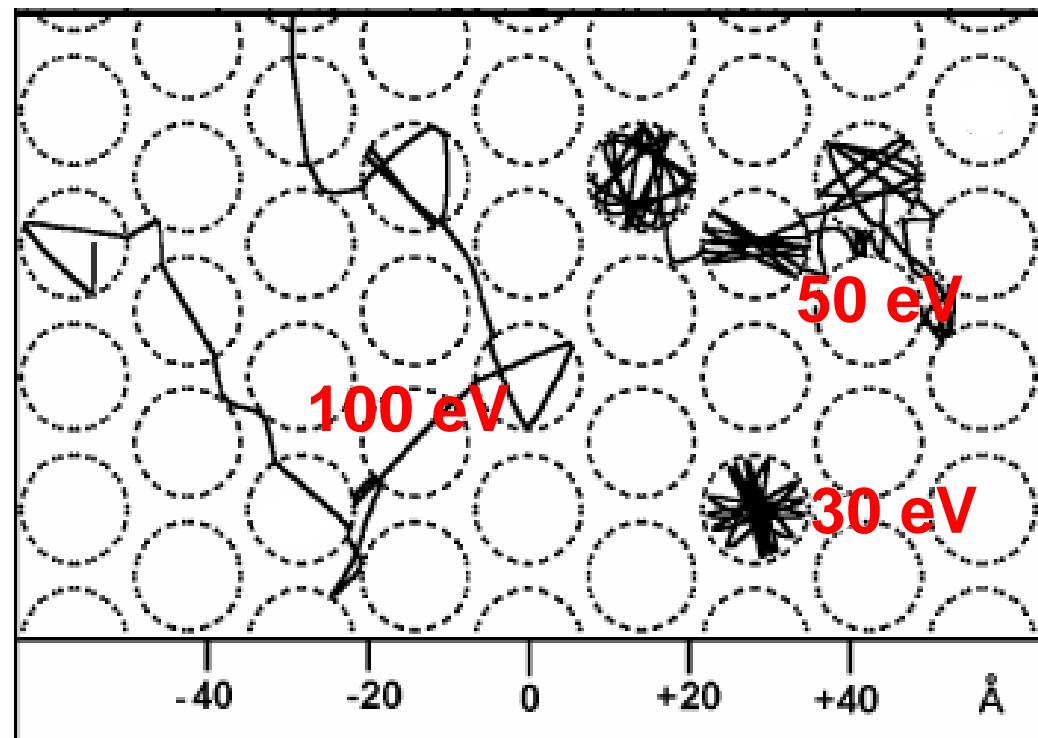
# Ion channelling through rope of armchair SWNTs<sub>(10,10)</sub>

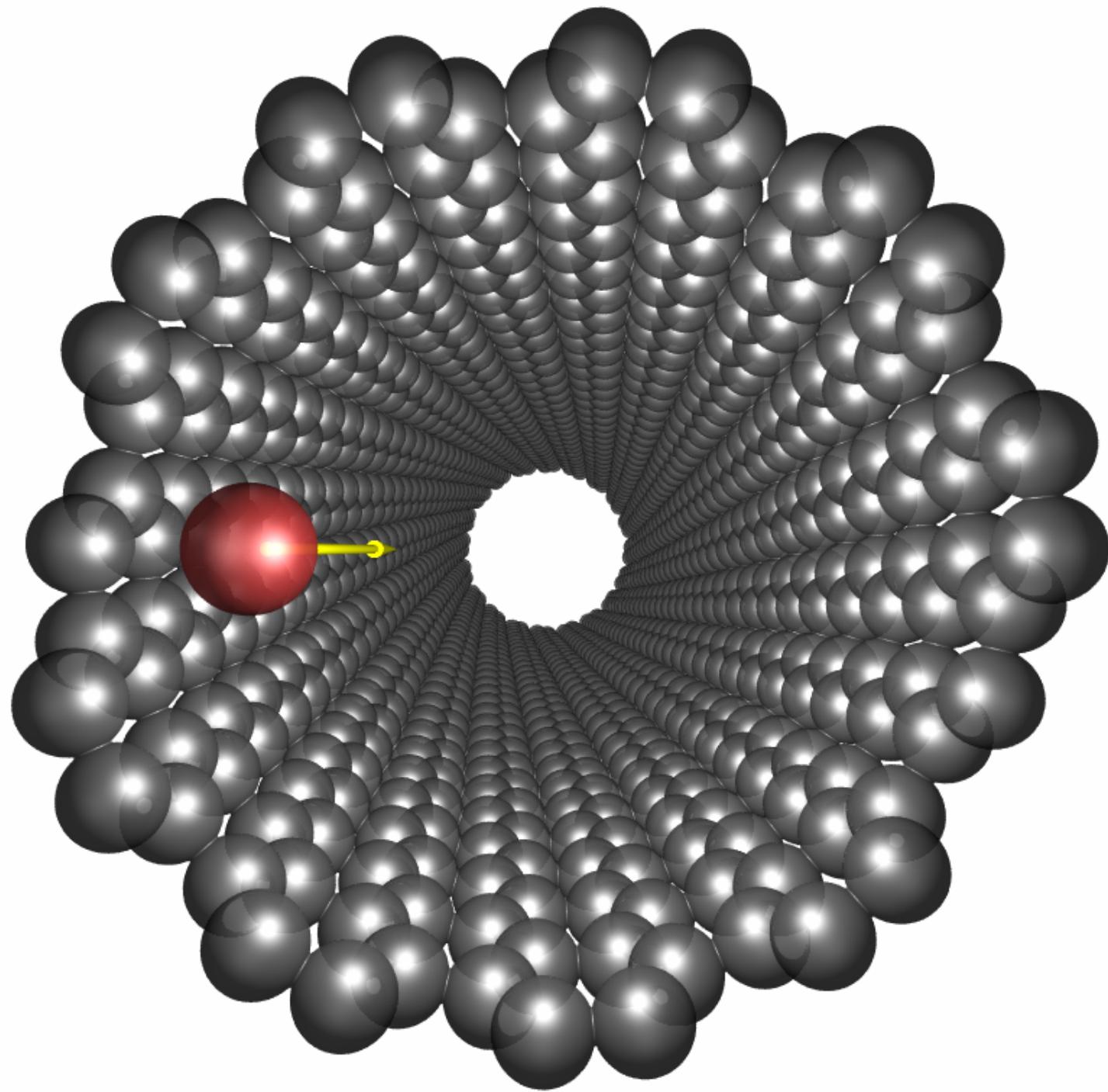
A.A. Greenenko and N.F. Shulga, *Nucl. Instr. Meth. B* 205 (2003) 767

Equi-potential surfaces (eV)



Ion trajectories with beam momentum 10 GeV/c and perpendicular energies 30, 50, and 100 eV

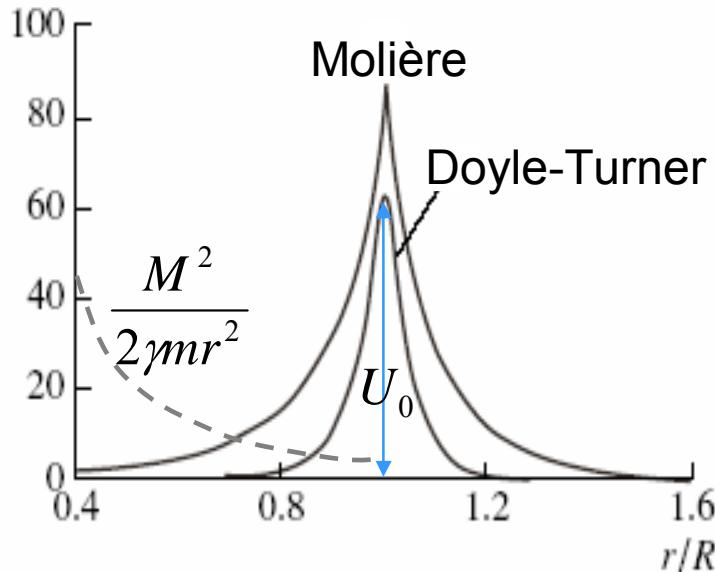




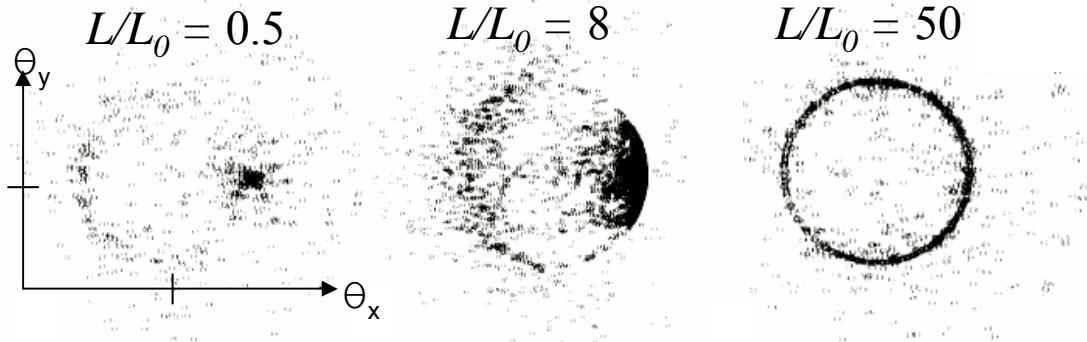
# Ion channelling through a straight chiral SWNT<sub>(11,9)</sub>

N.K. Zhevago and V.I. Glebov, *Phys. Lett. A* 250 (1998) 360 & 310 (2003) 301

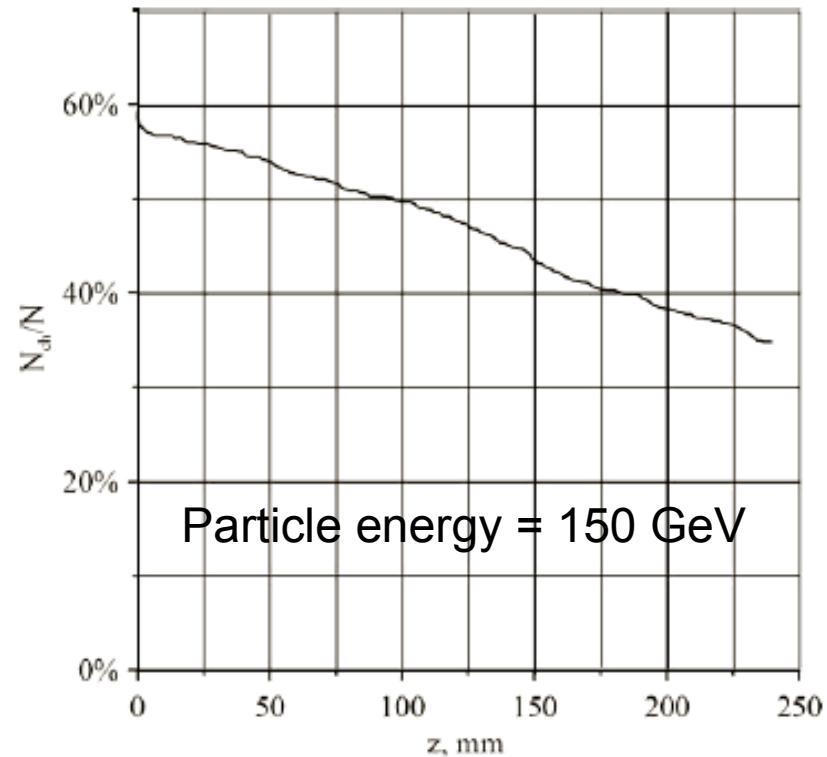
$U$ , eV Axially symmetric potential



Angular distributions of GeV ions for incident angles:  $\theta_{0x} = \theta_L/2$ ,  $\theta_{0y} = 0$



Removal of ions due to dechanneling



$$\theta_L = \sqrt{2U_0/E}$$

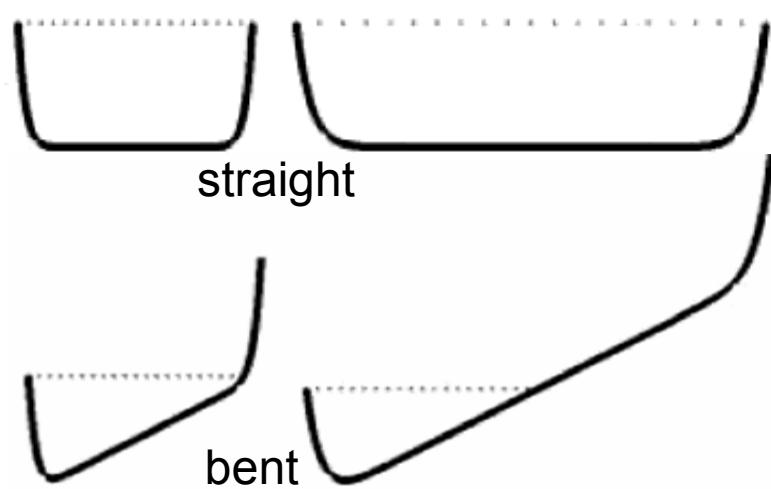
$$L_0 \equiv d/2\theta_L$$

# Optimal nanotube diameter for GeV proton beam steering in bent chiral SWNTs

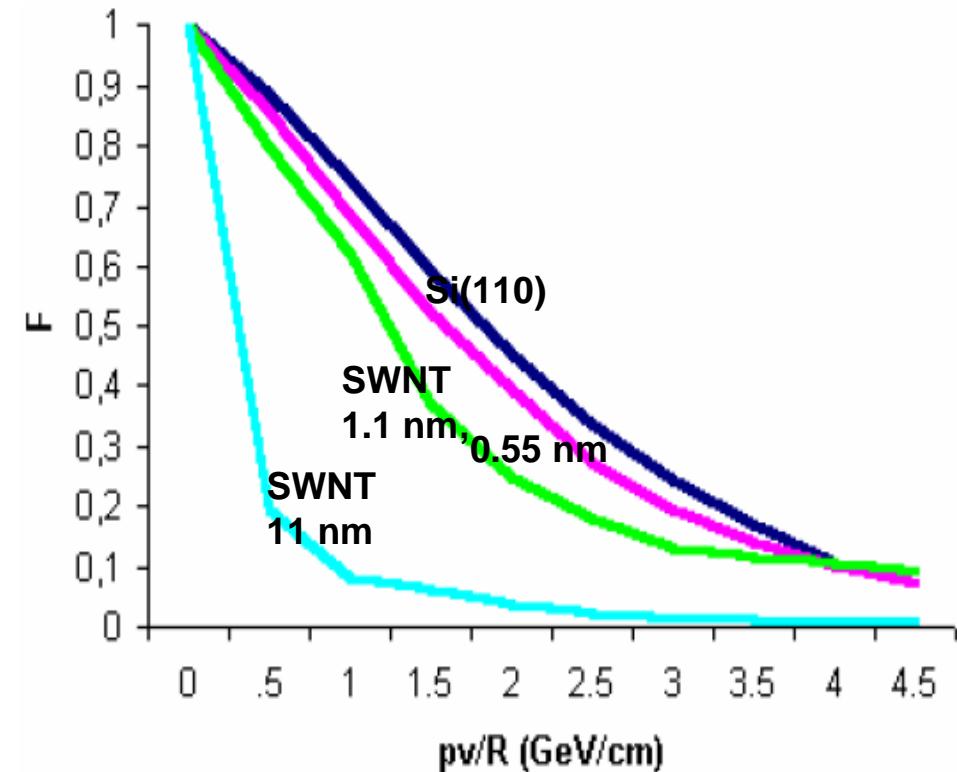
V.M. Biryukov and S. Bellucci, *Phys. Lett. B* 542 (2002) 111

Effective potentials inside narrow and wide SWNTs

$$U_{eff}(x) = U(x) + \frac{pv}{R} x$$



Fractions of channelled protons vs nanotube curvature  $pv / R$  for: Si(110) crystal channel and three SWNTs with different diameters

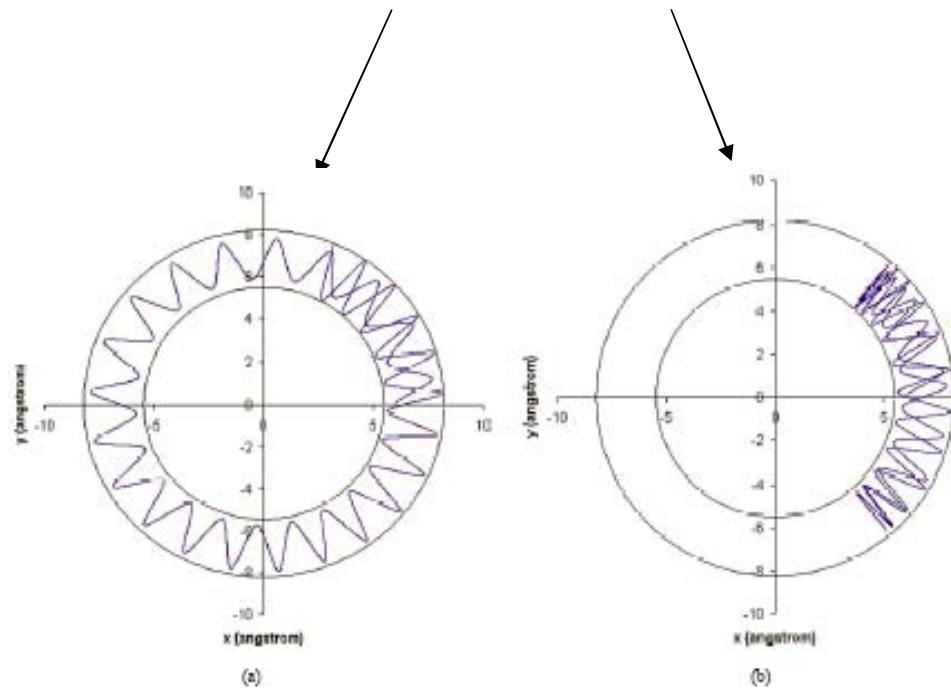


**Conclusion:** wide SWNTs are not more effective for beam steering

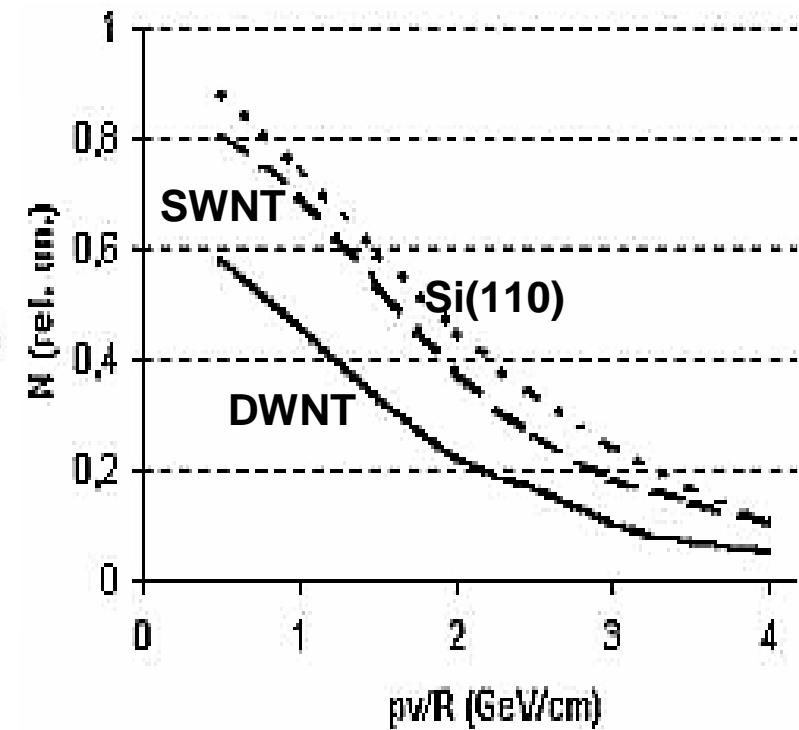
# GeV proton beam steering in bent chiral DWNTs

S. Bellucci *et al.*, *Phys. Lett. B* 608 (2005) 53

Proton trajectories between the walls  
in (a) **straight** and (b) **bent** DWNT



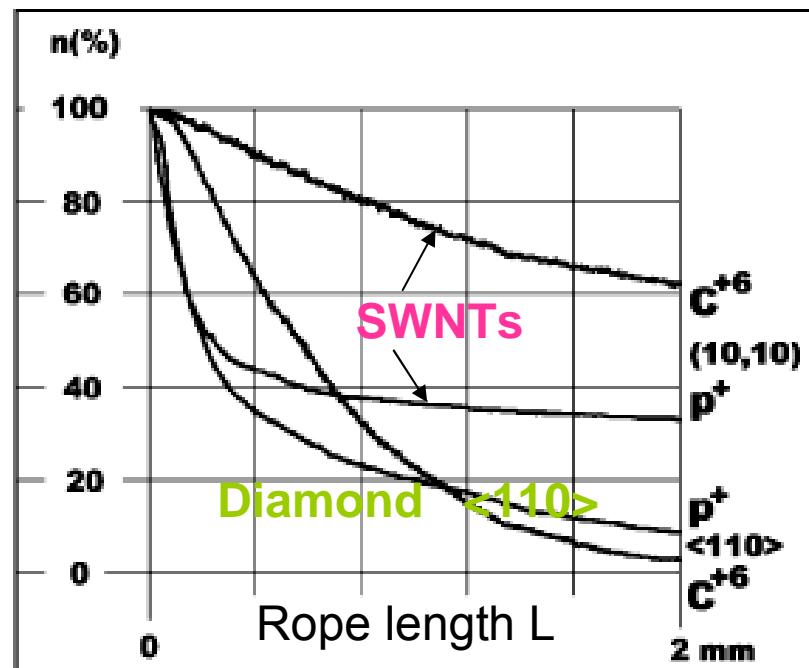
Fractions of protons channelled  
through: Si(110) crystal channel,  
SWNT with diameter 0.55 nm,  
and a DWNT



# Deflected beam fractions in bent ropes of SWNTs

## Rope of armchair SWNTs(10,10)

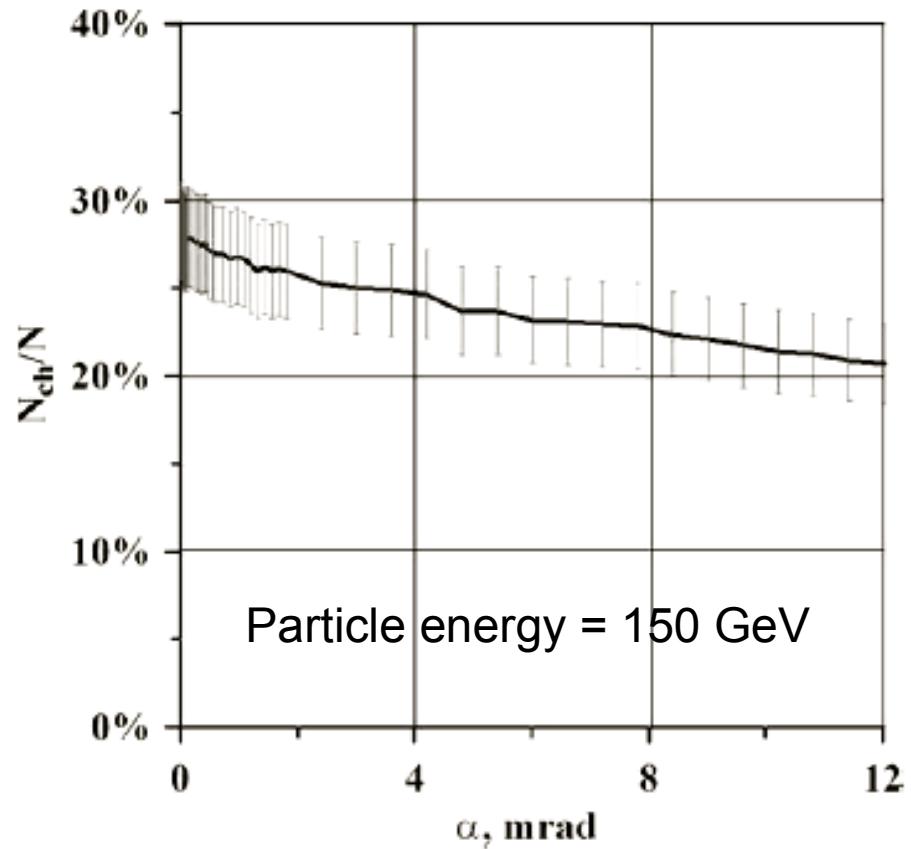
A.A. Greenenko and N.F. Shulga,  
*Nucl. Instr. Meth. B* 205 (2003) 767



Curvature radius  $R = 20$  cm  
Beam momentum=10 GeV/c

## Rope of chiral SWNTs(11,9)

N.K. Zhevago and V.I. Glebov,  
*Phys. Lett. A* 310 (2003) 301



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## Theory of rainbows in short ropes of SWNTs

- Scattering angles depend on impact parameters ( $x_0, y_0$ ) and length L

$$\Theta_x = \Theta_x(x_0, y_0; L), \quad \Theta_y = \Theta_y(x_0, y_0; L)$$

- In the small-angle approximation for short nanotubes, the differential cross section for ion transmission

$$\sigma = 1/|J|$$

- $J = \partial_x \Theta_x \partial_y \Theta_y - \partial_x \Theta_y \partial_y \Theta_x$  is the Jacobian of the mapping

$$(x_0, y_0) \rightarrow (\Theta_x, \Theta_y)$$

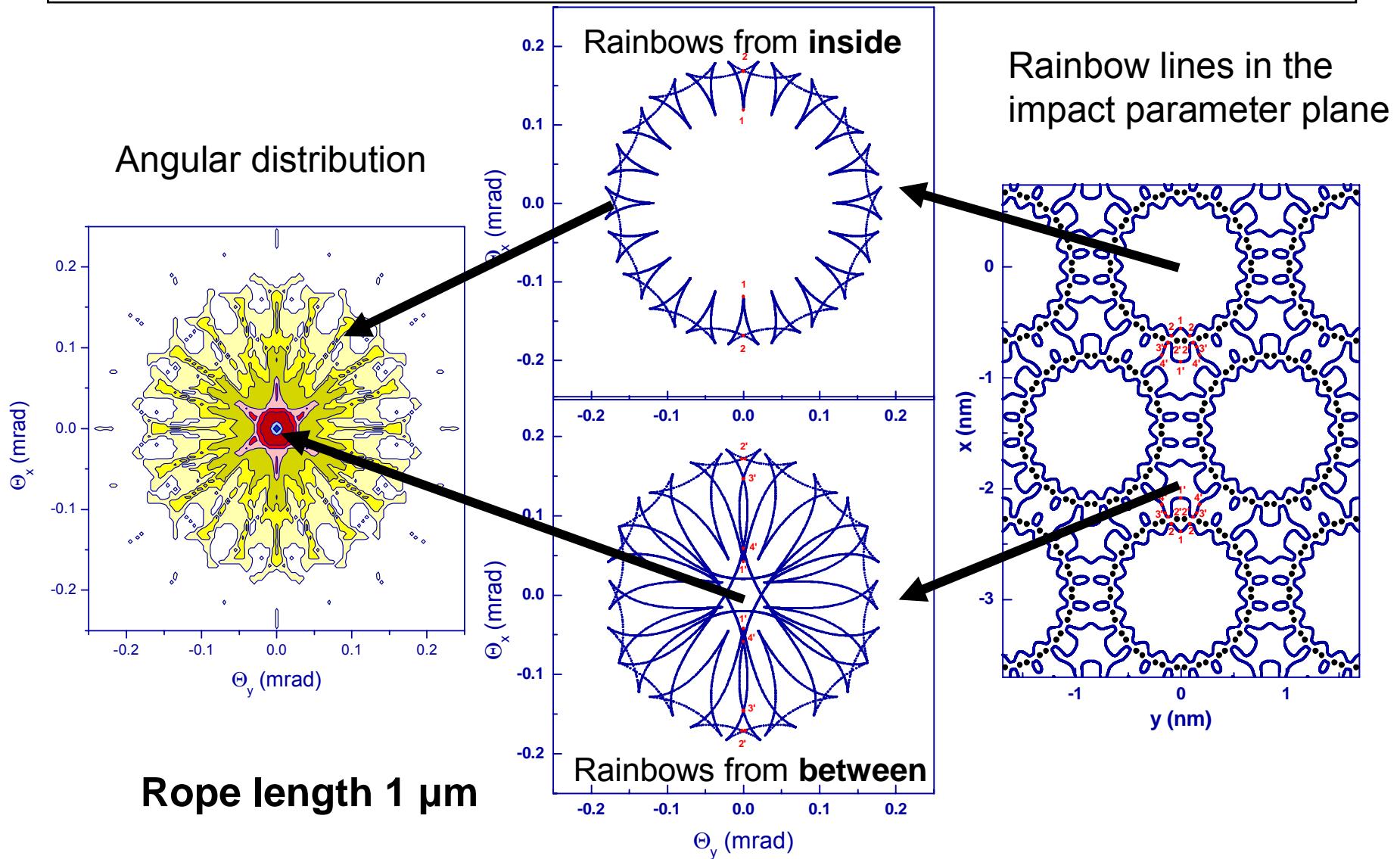
- Rainbow lines in the impact parameter plane are defined by

$$J(x_0, y_0; L) = 0$$

- Total potential is sum over all atomic rows on all nanotubes in the rope
- Could be used for precise measurement of electron density in nanotubes

# Rainbow effect after 1GeV proton channelling through a short rope of armchair SWNTs(10,10)

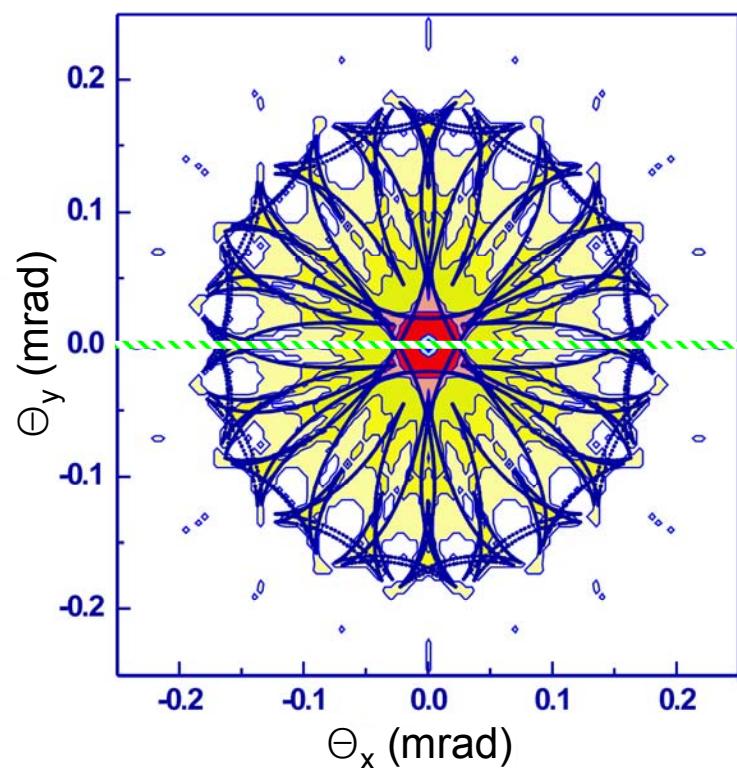
S. Petrovic *et al.*, *Eur. Phys. J. B* 44 (2005) 41



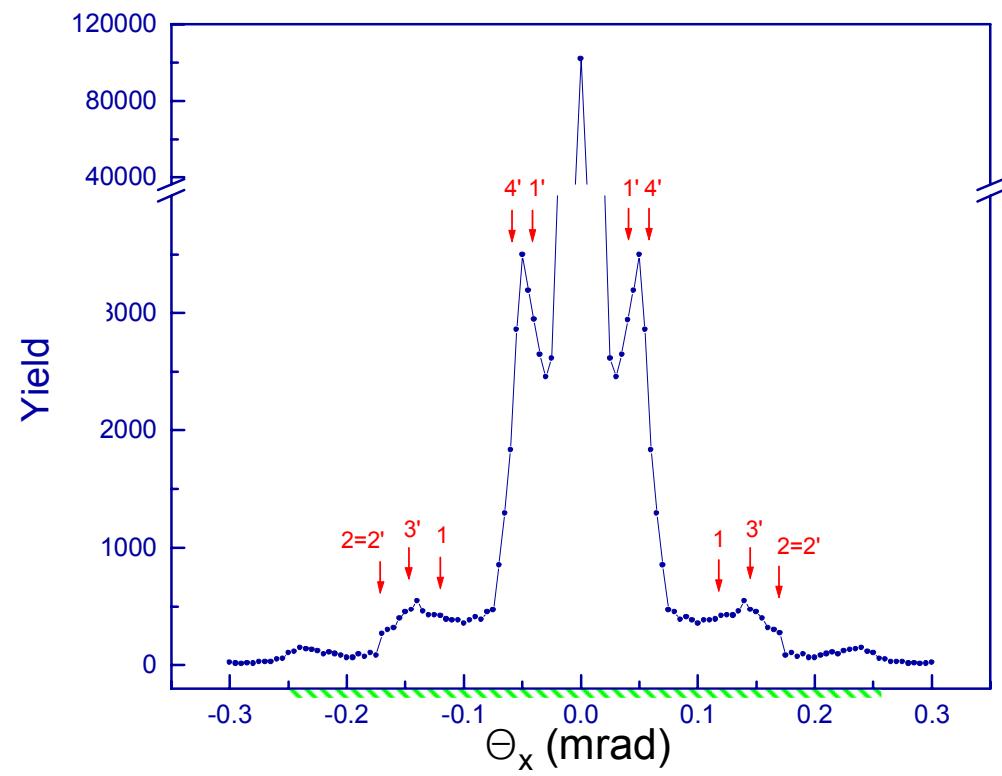
# Rainbow effect after 1GeV proton channelling through a short rope of armchair SWNTs(10,10)

S. Petrovic *et al.*, *Eur. Phys. J. B* 44 (2005) 41

Angular distribution  
with rainbow lines



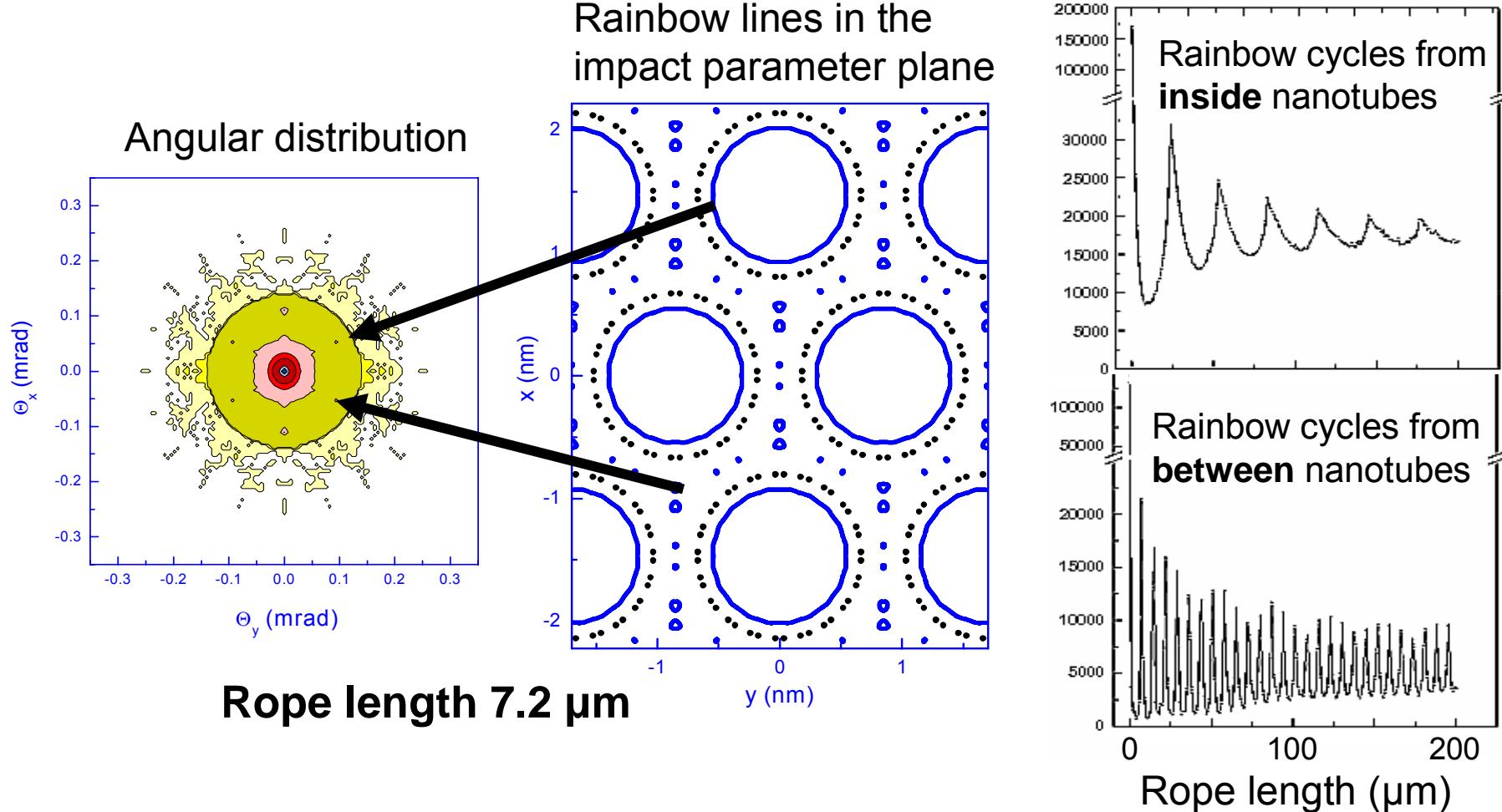
Yield of protons along  $\Theta_x$  line



**Rope length 1  $\mu$ m**

# Rainbow effect after 1GeV proton channelling through longer ropes of armchair SWNTs(10,10)

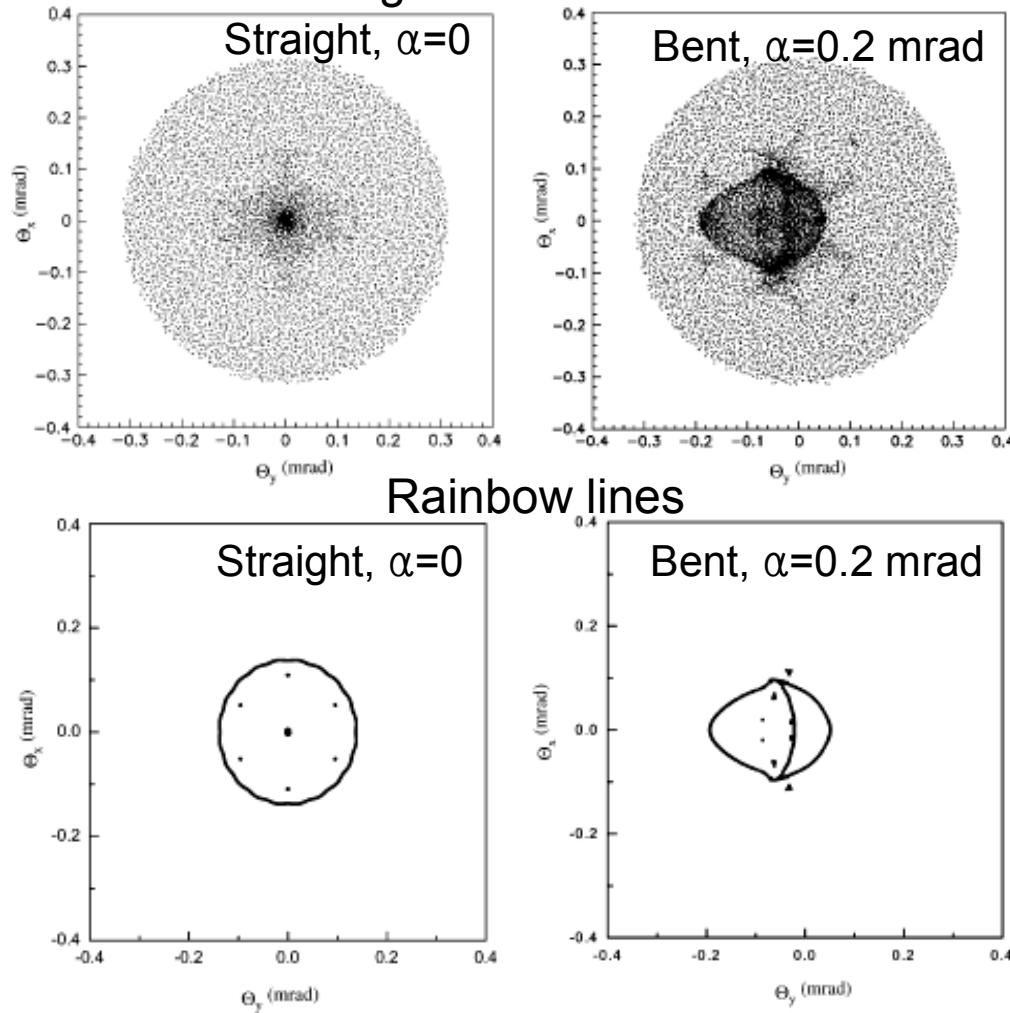
S. Petrovic *et al.*, *Nucl. Instr. Meth. B* 234 (2005) 78



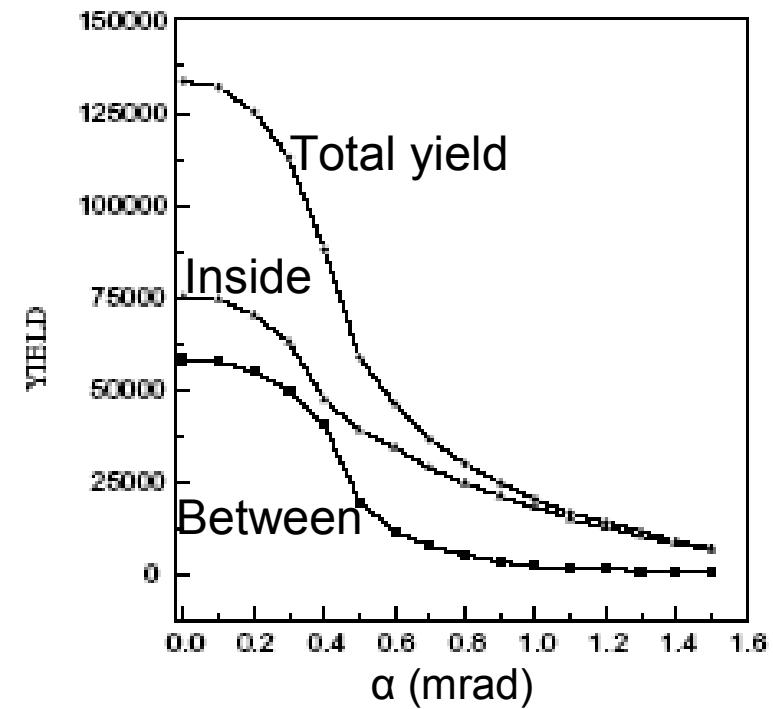
# Channeling of 1 GeV protons through a bent rope of armchair SWNTs (10,10)

N. Neskovic *et al.*, *Nucl. Instr. Meth. B* 230 (2005) 106

Angular distributions



Yields of protons transmitted inside and between nanotubes vs bending angle in 7  $\mu\text{m}$  rope

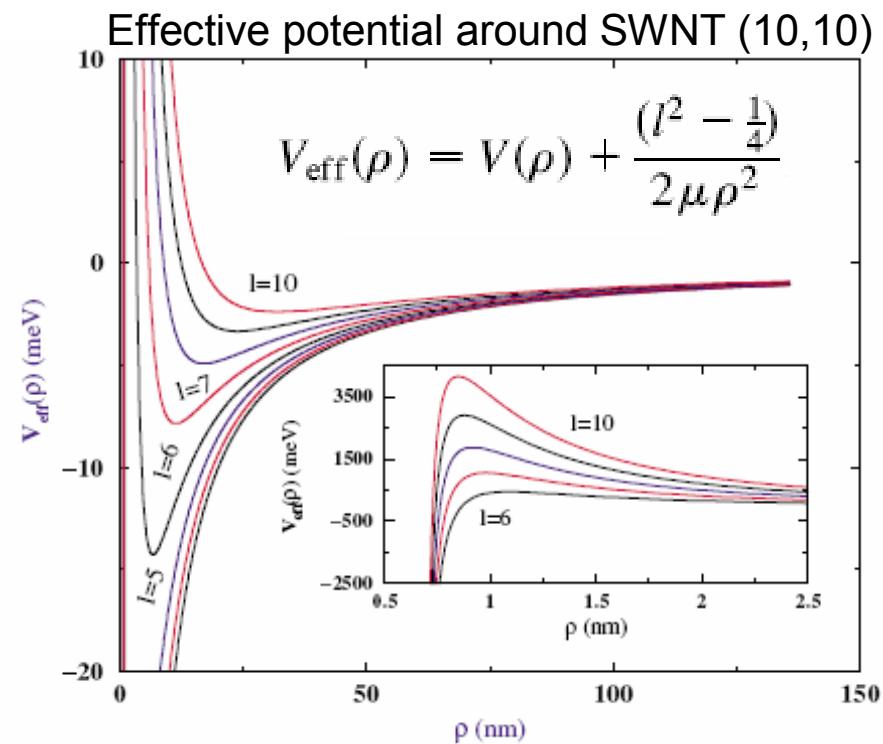
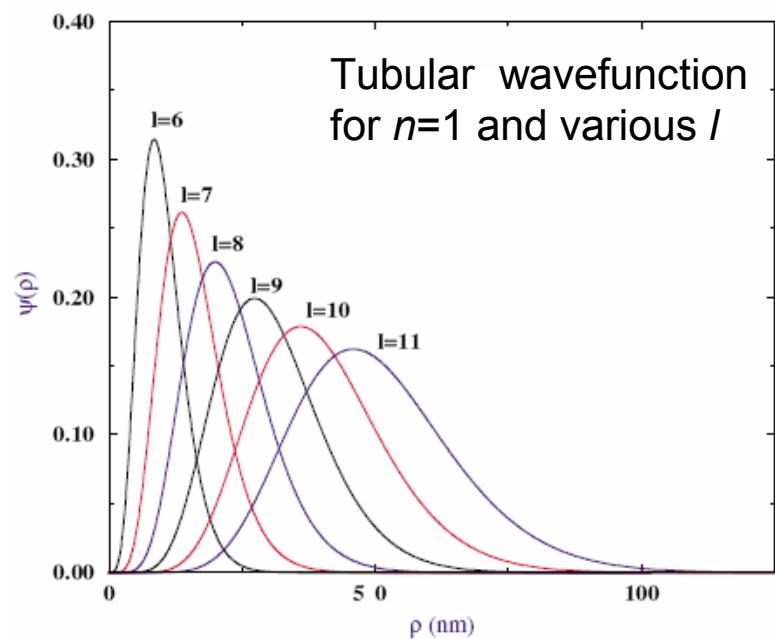
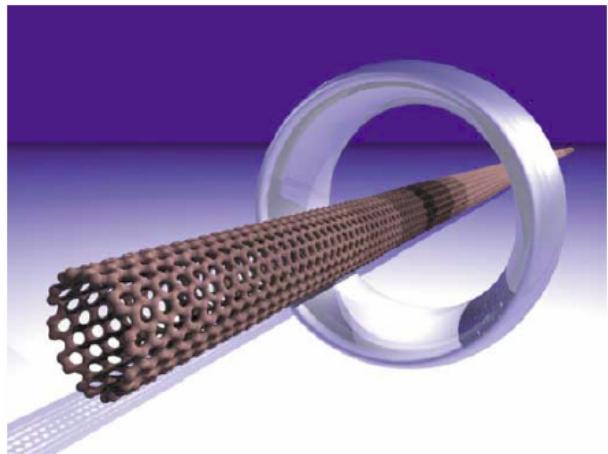


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# Electron image states around carbon nanotubes

Theoretical prediction: B.E. Granger *et al.*, *Phys. Rev. Lett.* 89 (2002) 135506



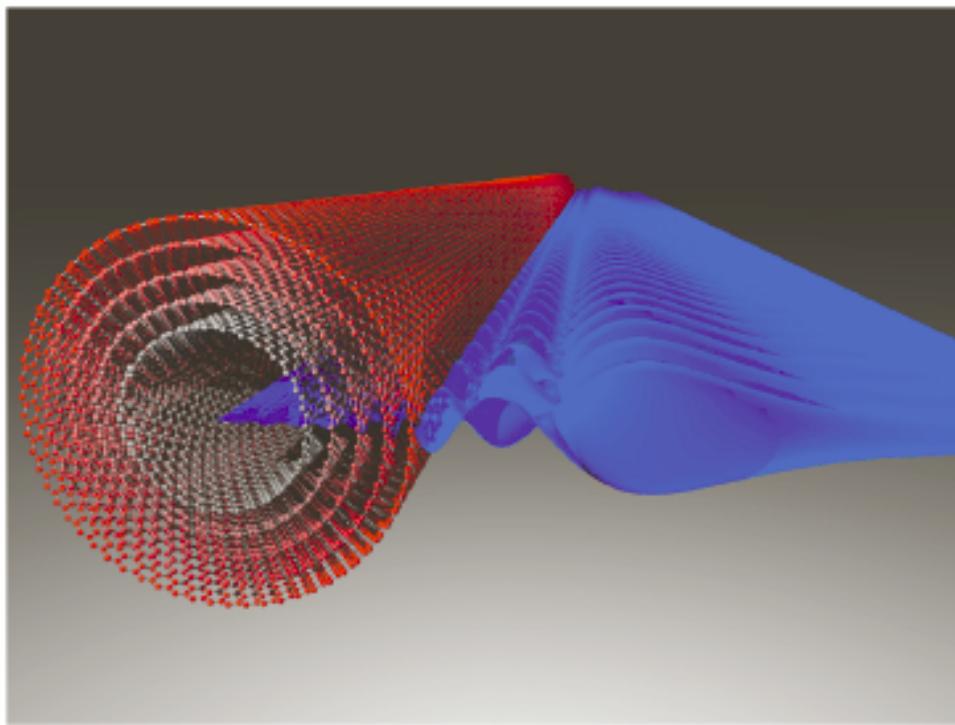
Approximate image potential

$$V(\rho_0) \approx \frac{2q^2}{\pi a} \sum_{n=1,3,5,\dots} \ln[(a/\rho_0)^n]$$

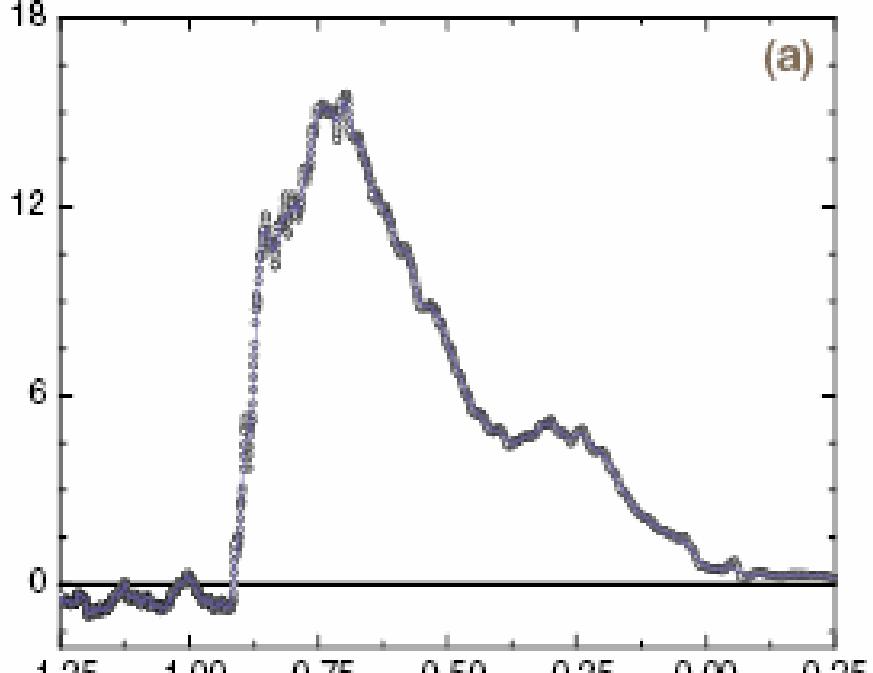
# Electron image states around carbon nanotubes

Experimental confirmation: M. Zamkov *et al.*, *Phys. Rev. Lett.* 93 (2004) 156803

Visualization of electron  
wavefunction with  $n=3, l=1$

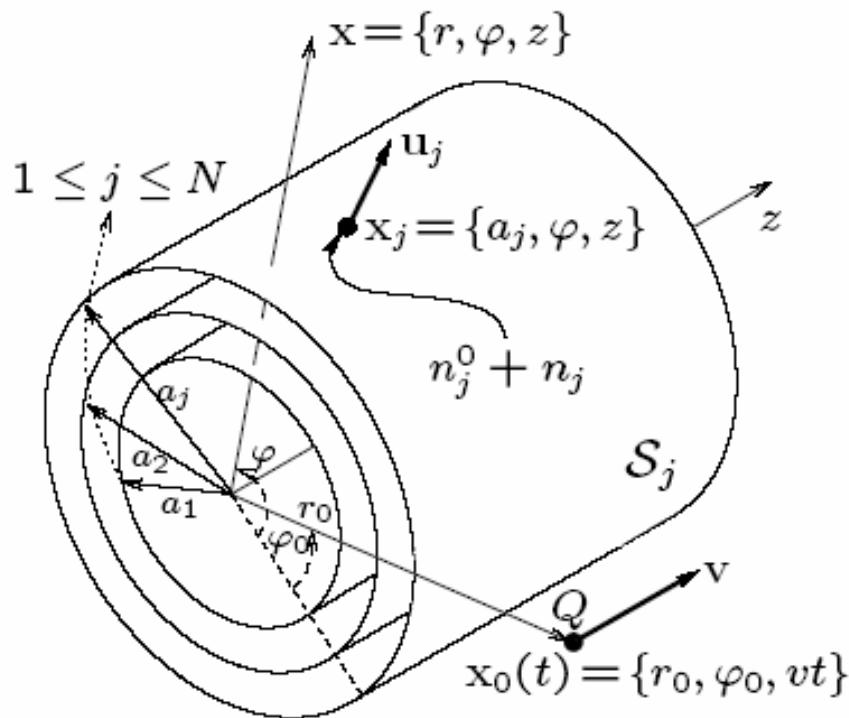


Photoelectron signal from image state



# 2D hydrodynamic model of electron response

D.J. Mowbray *et al.*, *Phys. Rev. B* 70 (2004) 195418



$$\frac{\partial n_j(x_j, t)}{\partial t} = -n_j^0 \nabla_j \cdot u_j(x_j, t)$$

$$\begin{aligned} \frac{\partial u_j(x_j, t)}{\partial t} = & \nabla_j \Phi(x, t)|_{r=a_j} - \frac{\alpha_j}{n_j^0} \nabla_j n_j(x_j, t) \\ & + \frac{\beta}{n_j^0} \nabla_j [\nabla_j^2 n_j(x_j, t)] - \gamma_j u_j(x_j, t) \end{aligned}$$

$$\Phi(x, t) = \frac{Q}{\|x - x_0(t)\|} - \sum_j \int_{S_j} d^2 x'_j \frac{n_j(x'_j, t)}{\|x - x'_j\|}$$

Stopping power

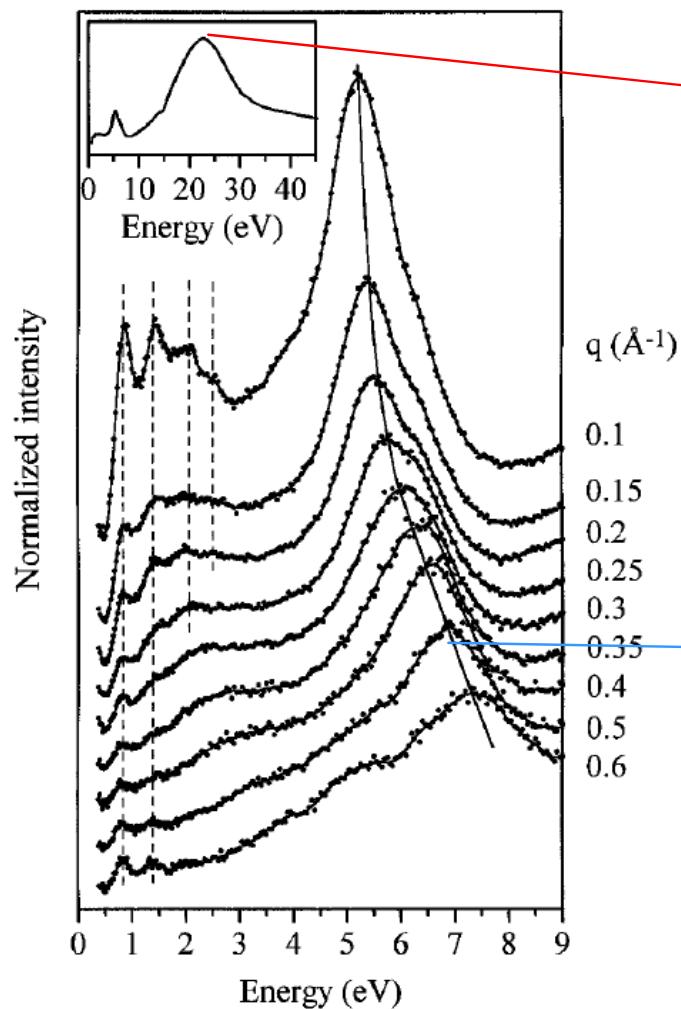
$$S = Q \frac{\partial \Phi_{ind}}{\partial z} \Big|_{x=x_0(t)}$$

Self-energy (image potential)

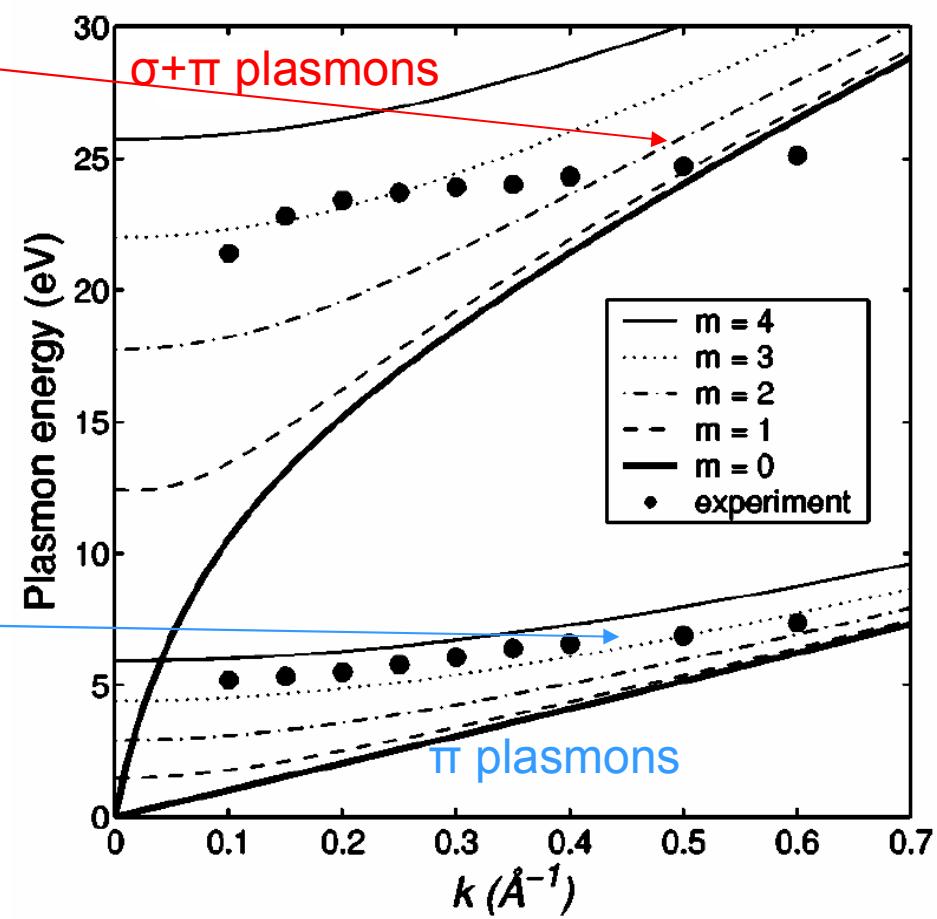
$$E_s = -\frac{Q}{2} \Phi_{ind} \Big|_{x=x_0(t)}$$

# Plasmon spectra: $\sigma$ and $\pi$ electrons on SWNT

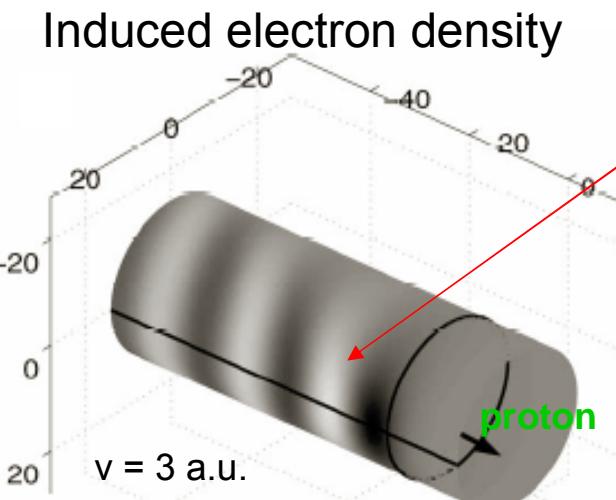
EELS experiment: T. Pichler *et al.*,  
*Phys. Rev. Lett.* 80 (1998) 4729



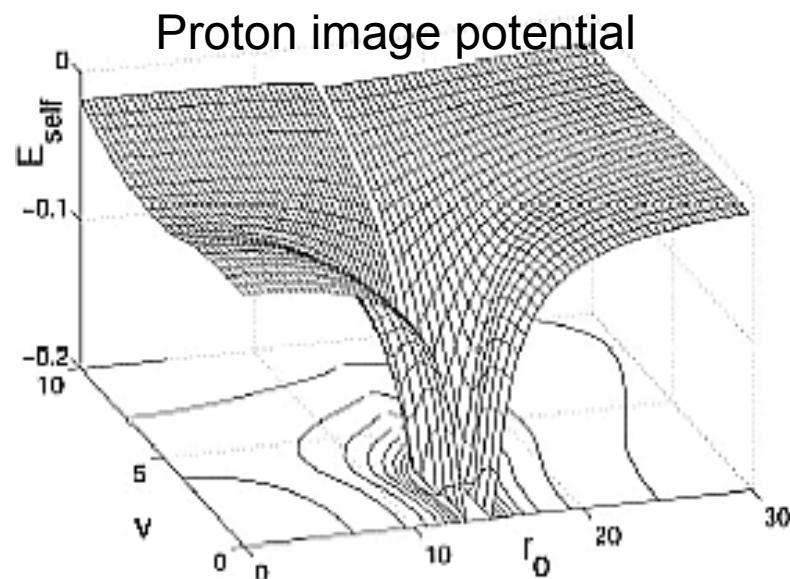
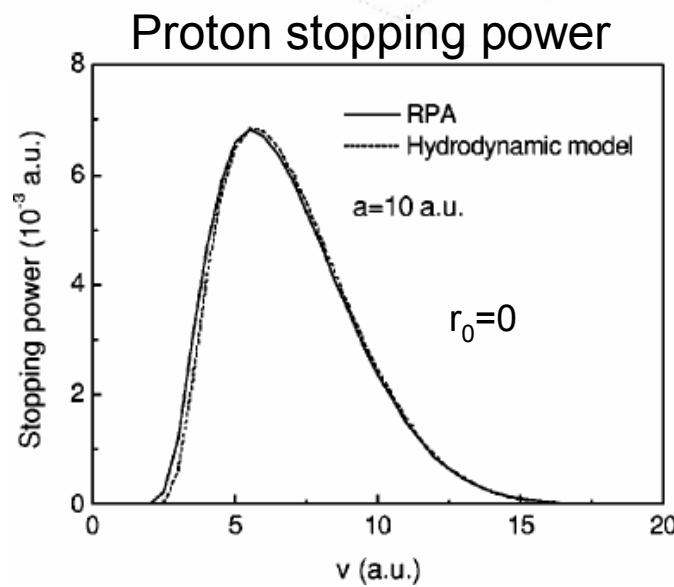
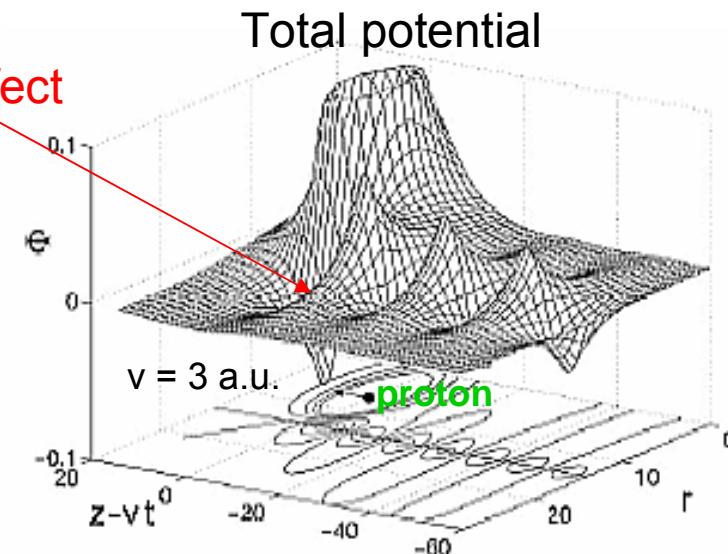
Theoretical plasmon dispersion:  
**Two-fluid model**



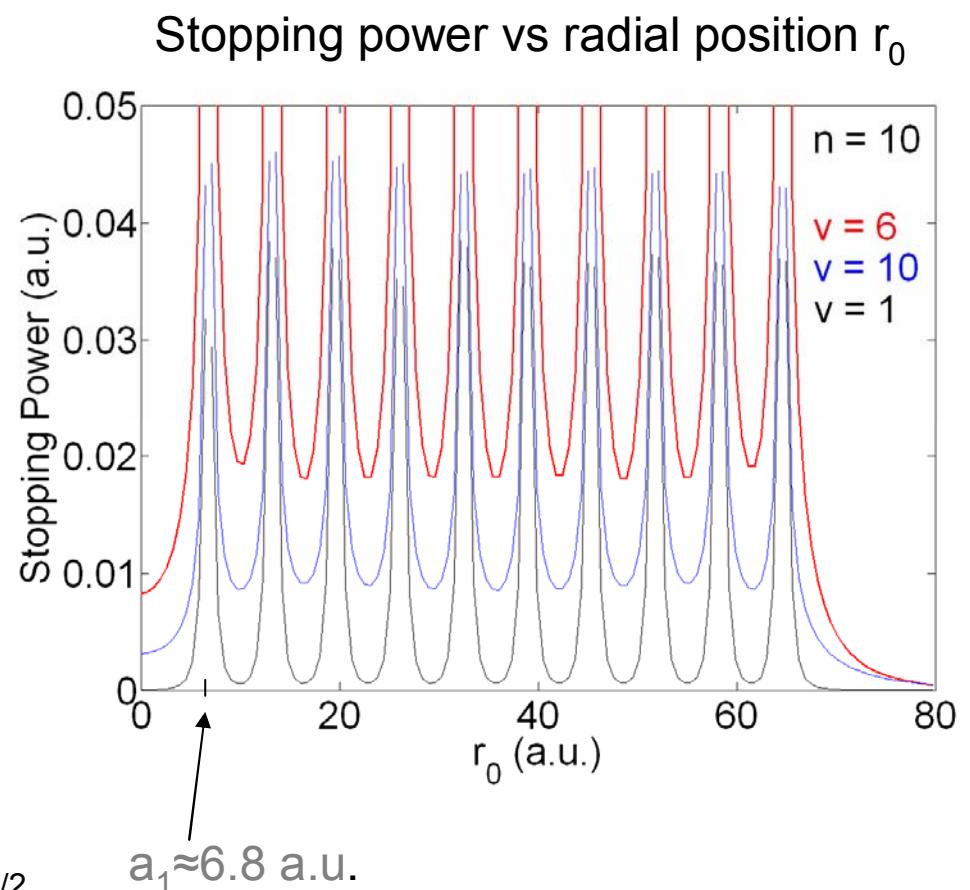
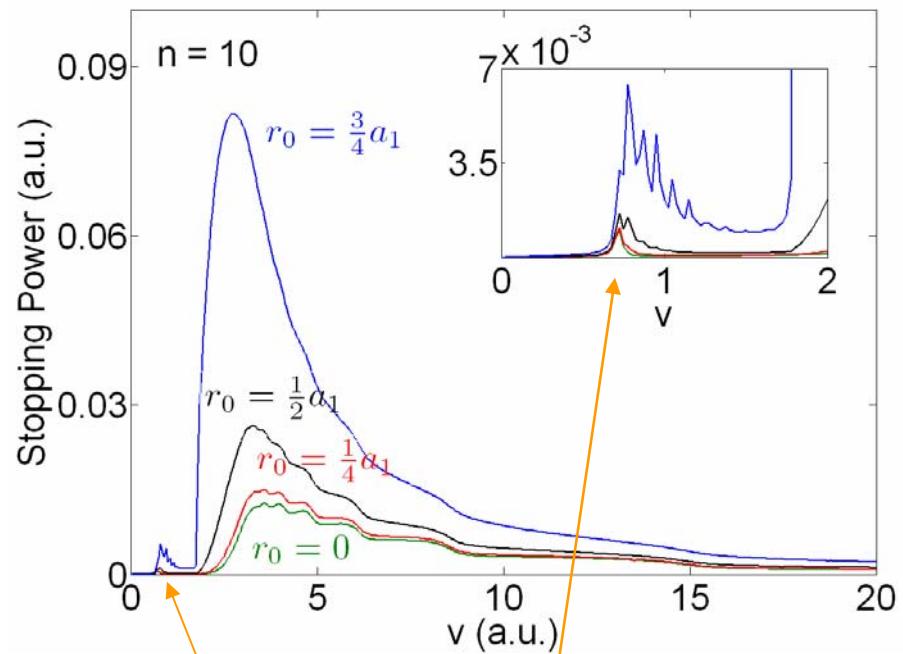
# Dynamic polarization of electrons on SWNT by proton



Wake effect

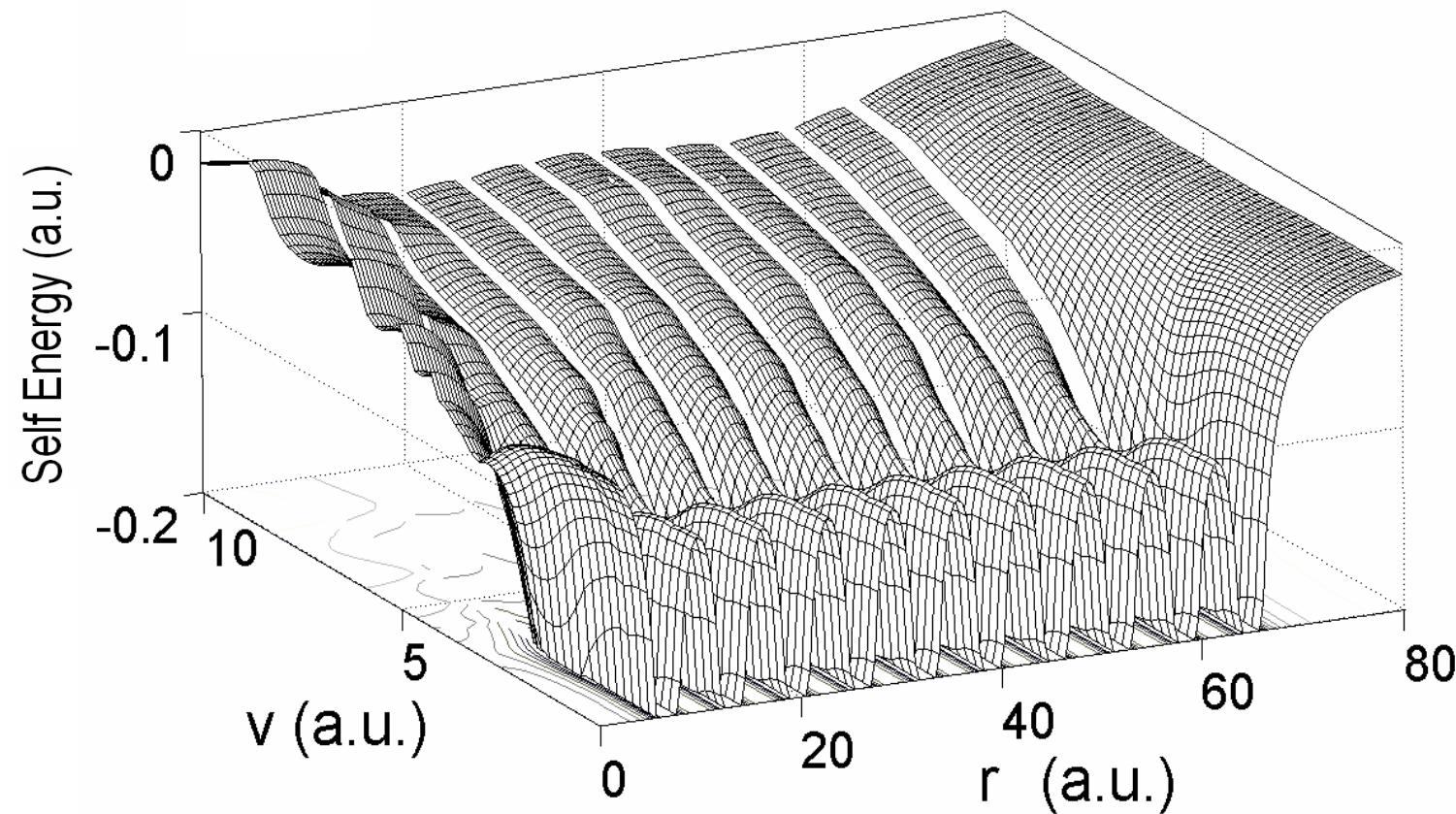


# Proton stopping power for MWNT with $n = 10$ walls



Calculations done with **two-fluid model**:  
 notice **low-speed features** due to quasi -  
 acoustic  $\pi$  plasmons having dispersion  
 $\omega_\pi \approx v_a k$  with acoustic speed  $v_a = (3\pi\sigma_0/8)^{1/2}$   
 $\approx 0.7$  a.u.. Is there a drift instability?

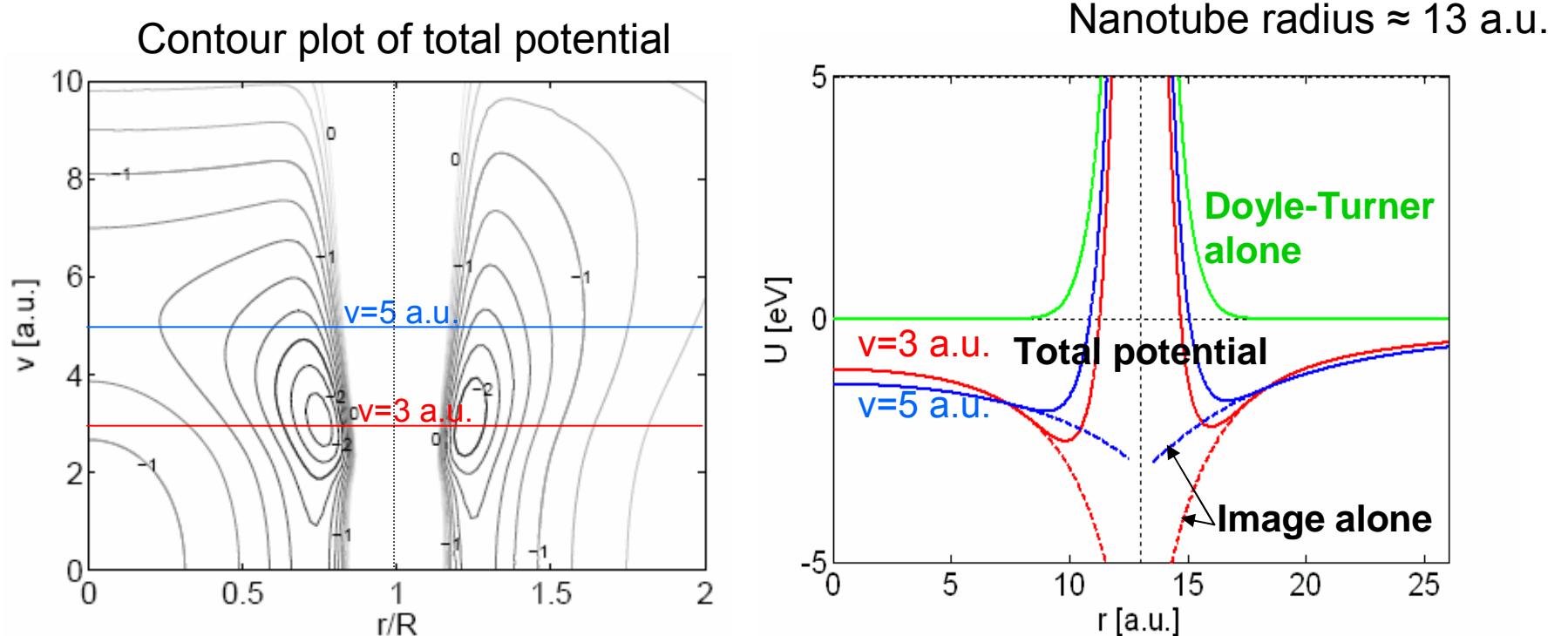
# Proton self energy (image potential) for MWNT with $n = 10$ walls (single-fluid model)



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# Total potential for proton moving parallel to a chiral SWNT<sub>(11,9)</sub> with image and Doyle-Turner potentials



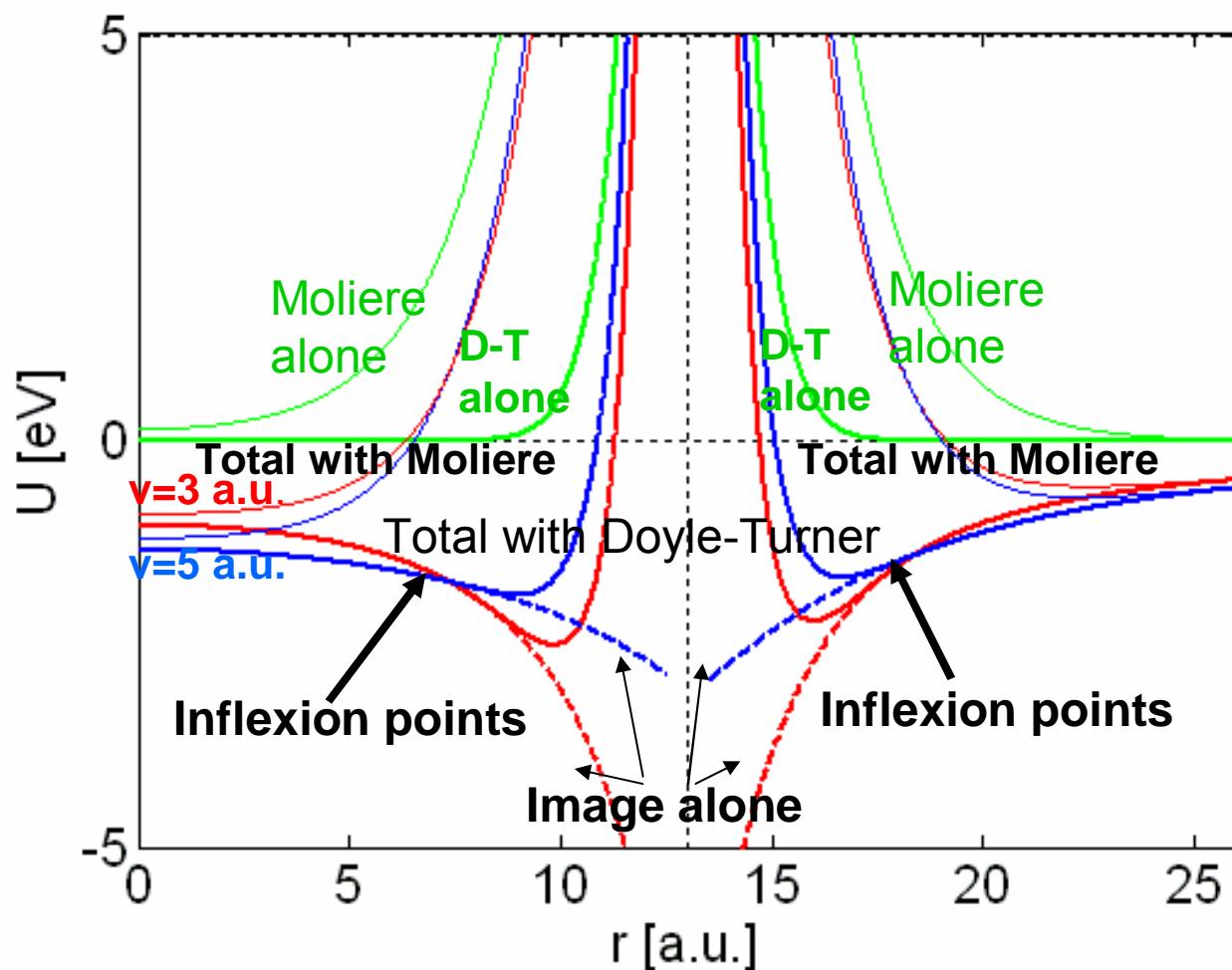
$$U_{im}(r) = \frac{Z_1^2}{\pi} \sum_{m=-\infty}^{\infty} P \int_0^{\infty} dk I_m^2(kr_<) K_m^2(kr_>) \frac{4\pi n_0 R (k^2 + m^2/R^2)}{(kv)^2 - \omega_m^2(k)}$$

$$\omega_m^2(k) = (k^2 + m^2/R^2) \left[ v_s^2 + 4\pi n_0 R I_m(kR) K_m(kR) \right], \quad r_< = \min(r, R), \quad r_> = \max(r, R)$$

$$U_{DT}(r) = 4\pi n_0 R Z_1 Z_2 \sum_{j=1}^4 a_j b_j^2 I_0(2b_j^2 R r) \exp \left[ -b_j^2 (r^2 + R^2) \right]$$

# Comparison of Doyle-Turner and Moliere potentials for proton moving parallel to SWNT<sub>(11,9)</sub> at v = 3 and 5 a.u.

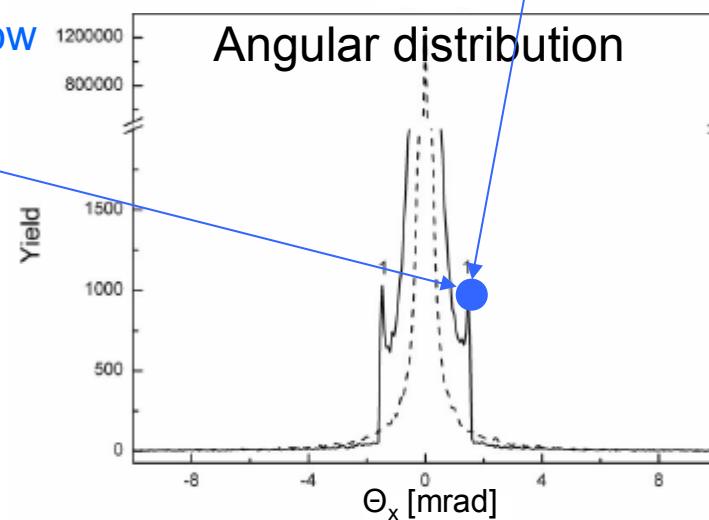
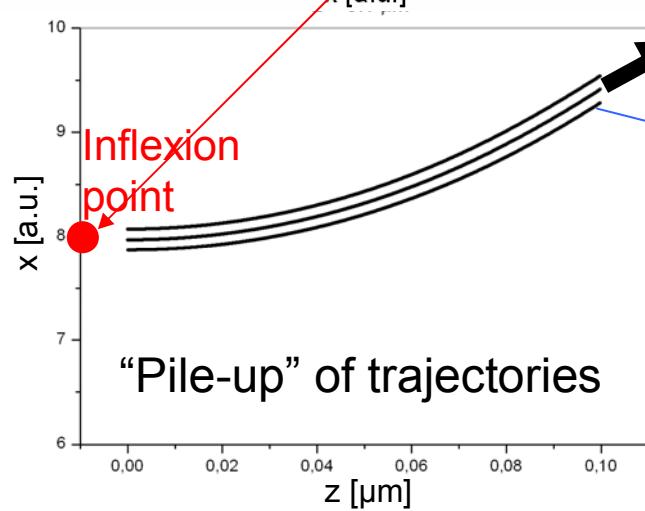
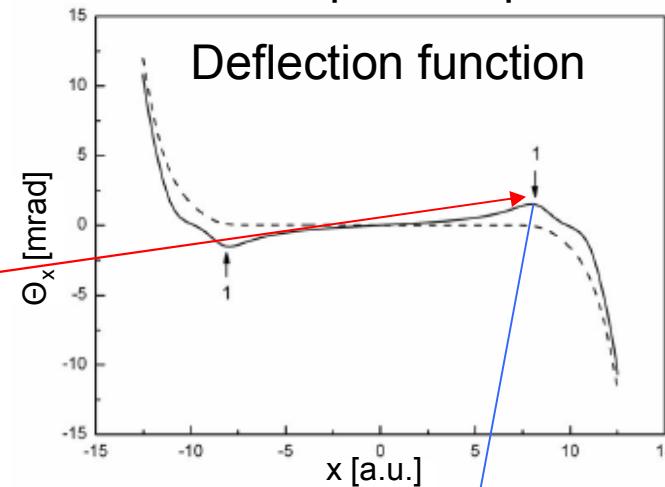
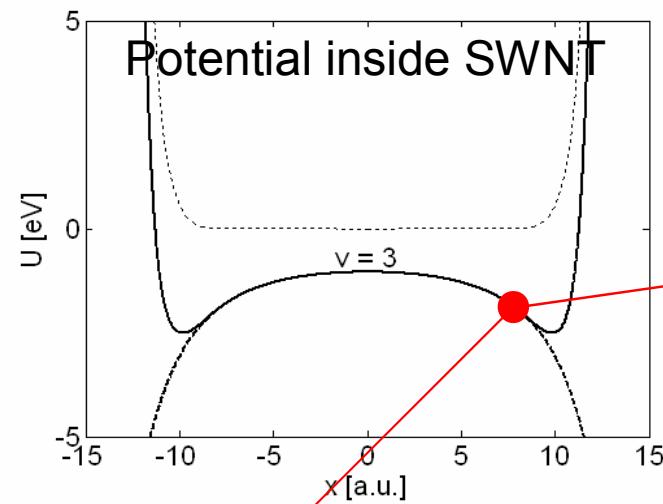
Nanotube radius  $\approx$  13 a.u.



# Rainbow effect for proton channelling in short chiral SWNT<sub>(11,9)</sub> with image & Doyle-Turner potentials

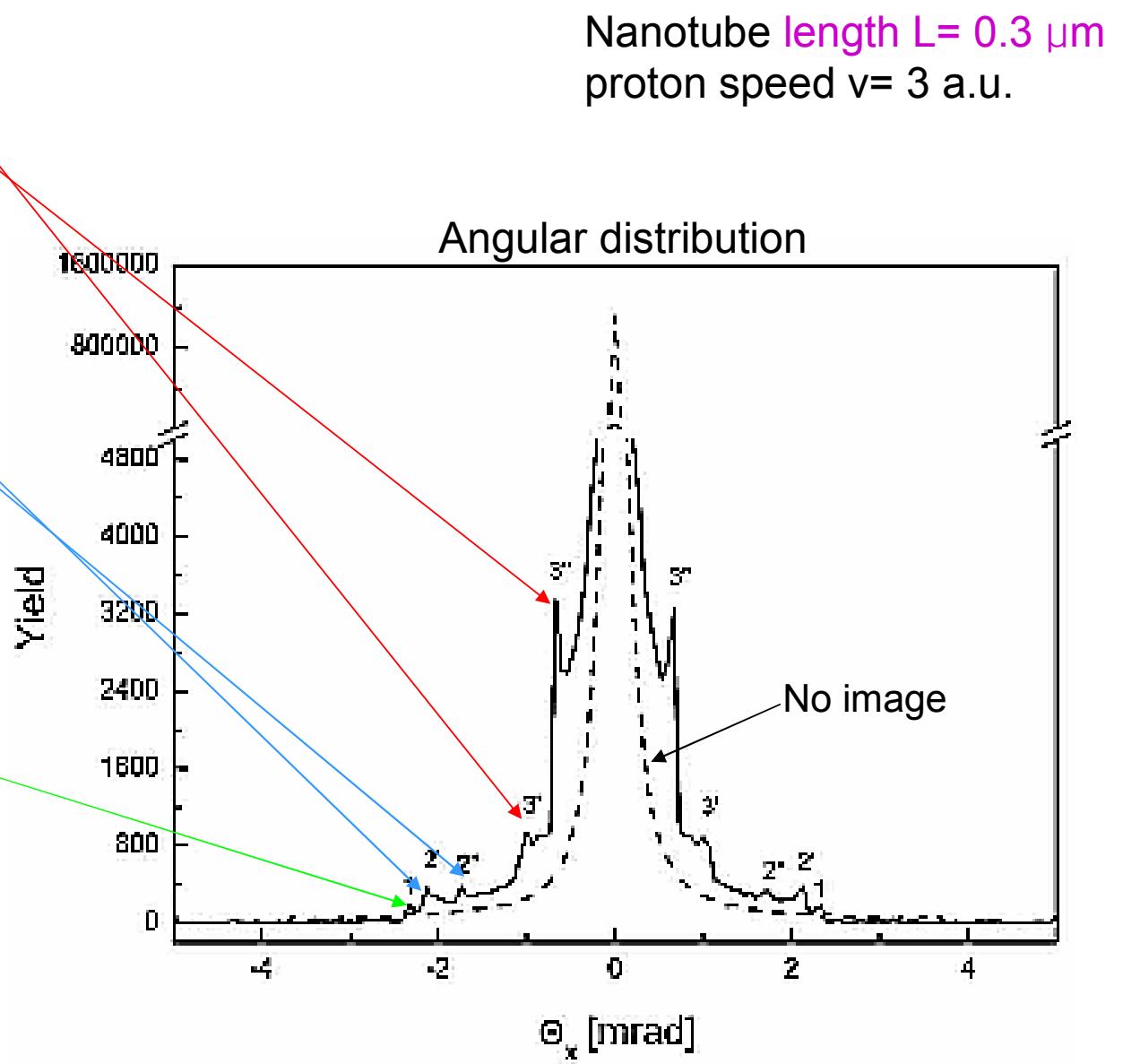
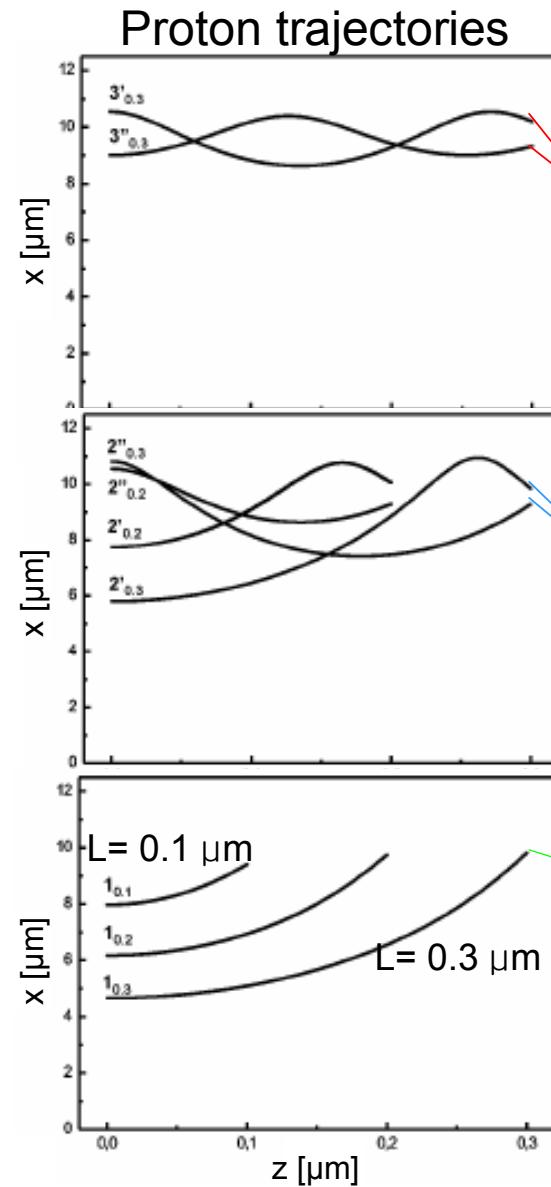
$$J = \left( \frac{L}{2E} \right)^2 \frac{1}{2r} \frac{d}{dr} \left[ \frac{dU(r)}{dr} \right]^2 = 0 \Rightarrow \sigma = \frac{1}{|J|} \rightarrow \infty$$

Nanotube length L = 0.1 μm  
proton speed v = 3 a.u.



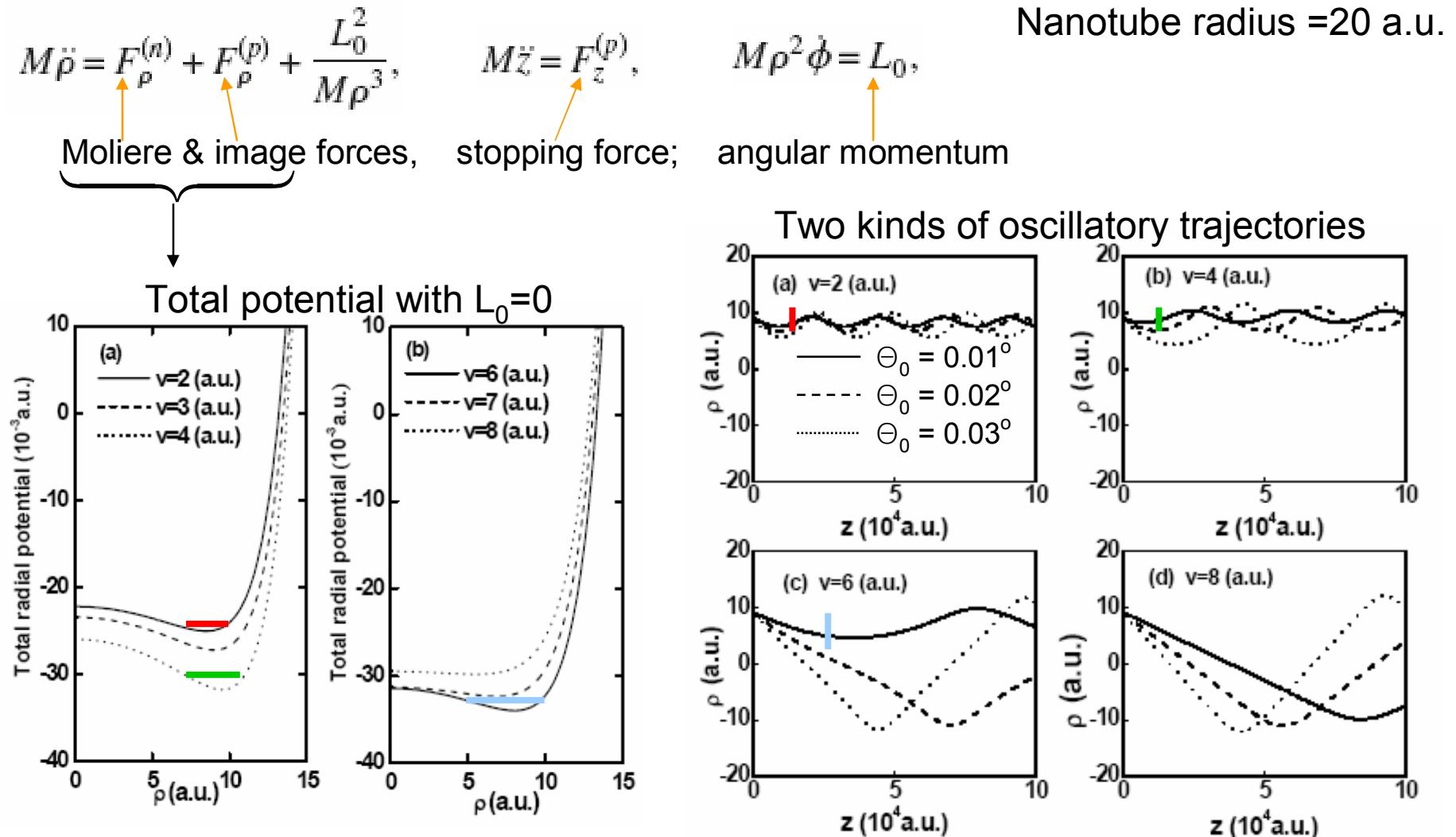
# Formation of multiple rainbows in chiral SWNT<sub>(11,9)</sub>

D. Borka *et al.*, *Phys. Rev. A*, in press (2006)



# Proton channelling through a wider & longer chiral SWNT with image and Moliere potentials

D.P. Zhou *et al.*, Phys. Rev. A 72 (2005) 23202

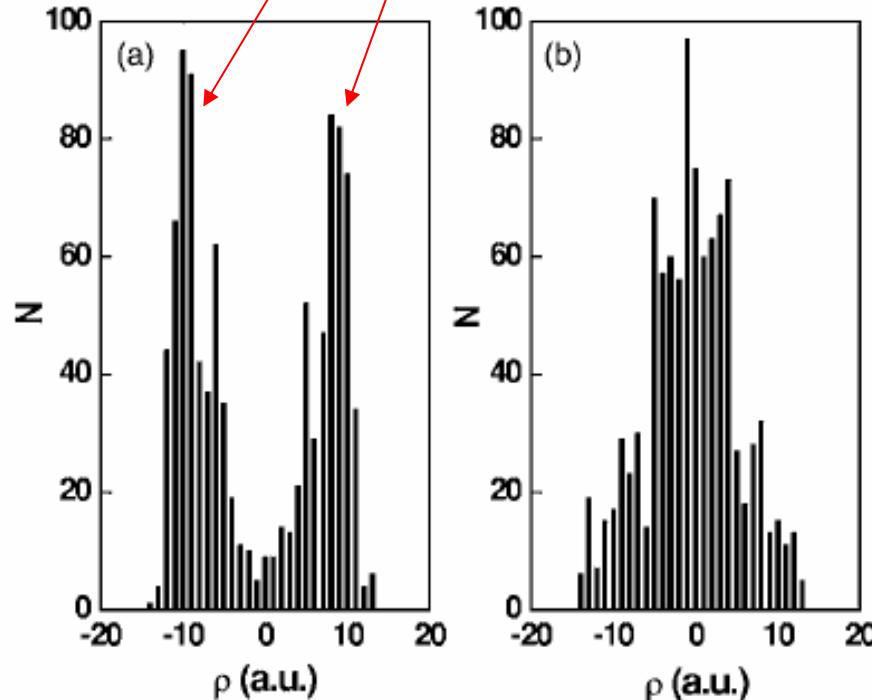


# Creation of hollow nano-beam of protons after channelling through a SWNT due to image force

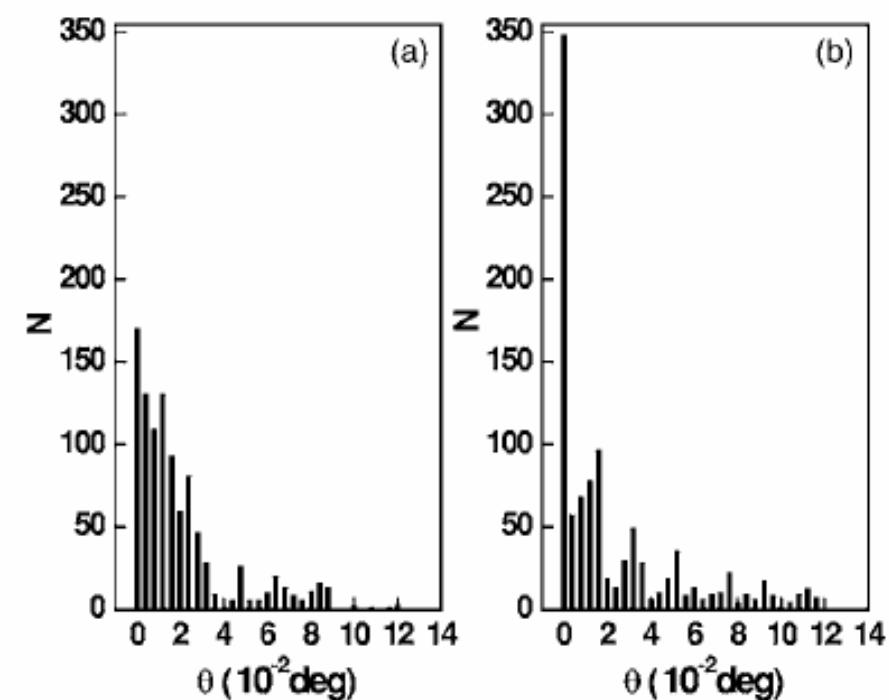
D.P. Zhou *et al.*, Phys. Rev. A 72 (2005) 23202

Proton speed = 4 a.u., NT radius = 20 a.u., NT length =  $10^5$  a.u.

Radial distributions of ion flux after channelling **with** and without image



Angular distributions after channelling **with** and without image interaction



# Coulomb explosions during H<sub>2</sub><sup>+</sup> channelling in SWNT

D.P. Zhou *et al.*, Phys. Rev. A 73 (2006) 33202

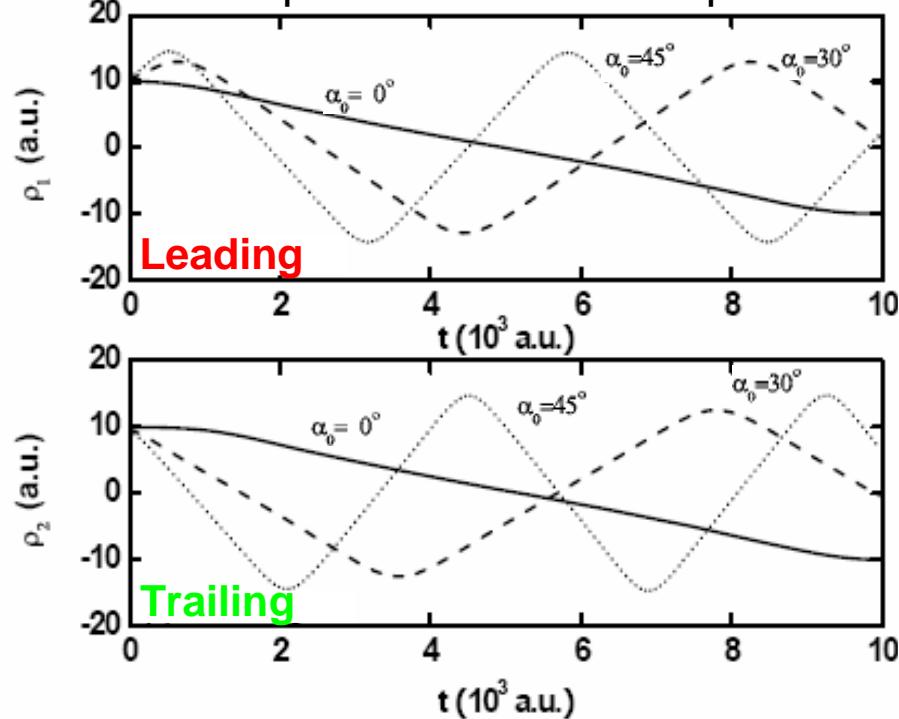
Solve classical equations of motion:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{u}_i, \quad M_i \frac{d\mathbf{u}_i}{dt} = \sum_{j(\neq i)=1}^2 \mathbf{F}_{ij}^{(c)} + \sum_{j=1}^2 \mathbf{F}_{ij}^{(p)} + \mathbf{F}_i^{(n)}$$

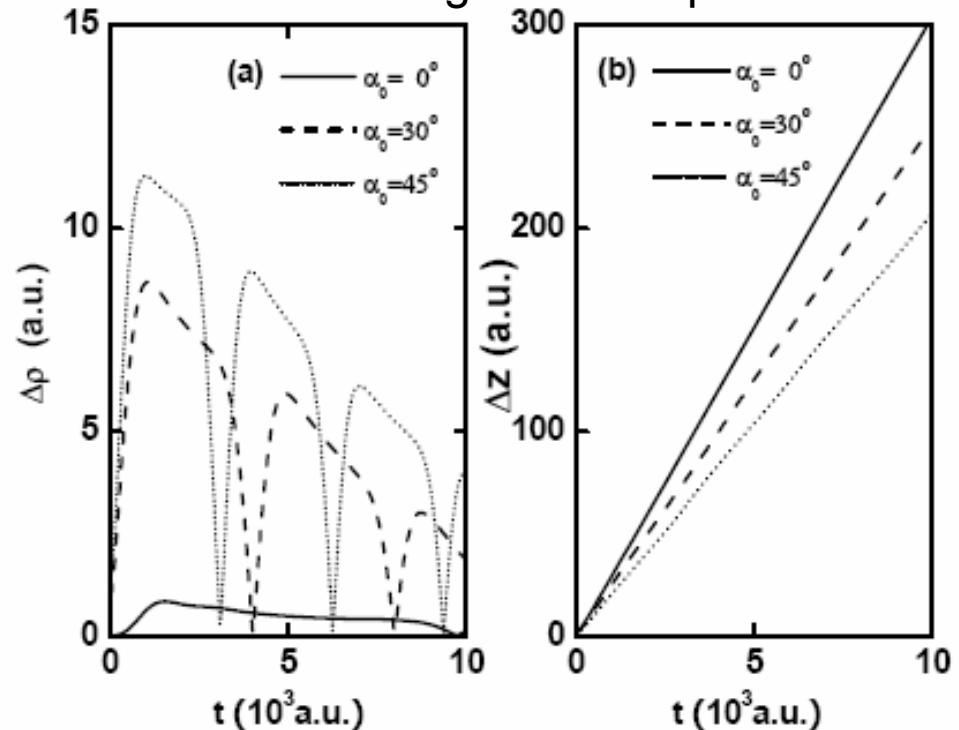
Molecule speed = 5 a.u. and  
alignment angles = 0°, 30°, 45°

Forces: Coulomb, polarization, Moliere

Radial positions of the two protons



Radial and longitudinal separations



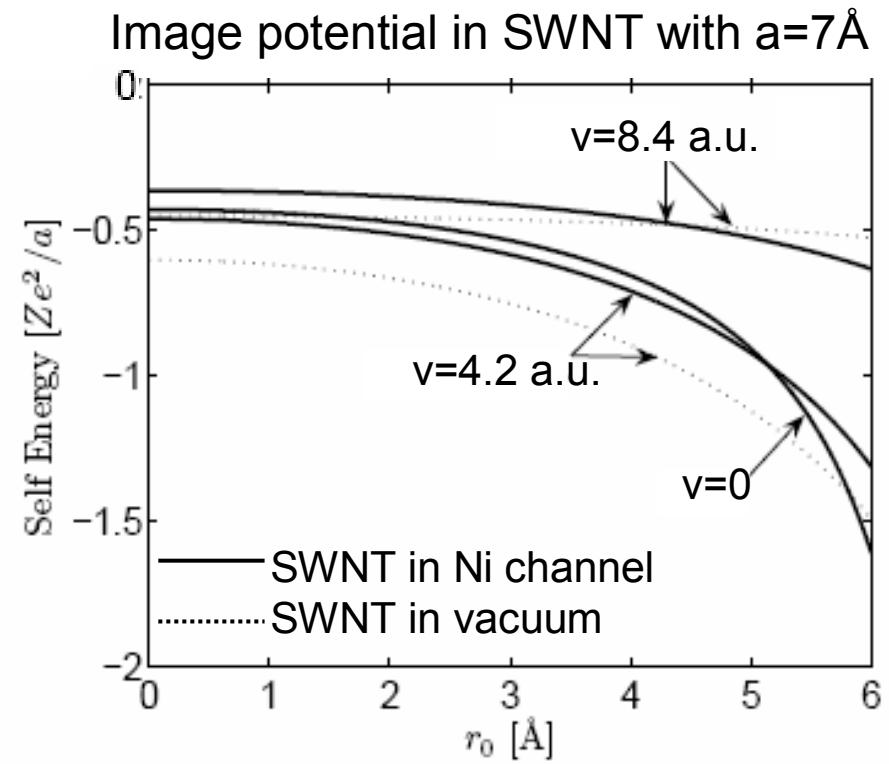
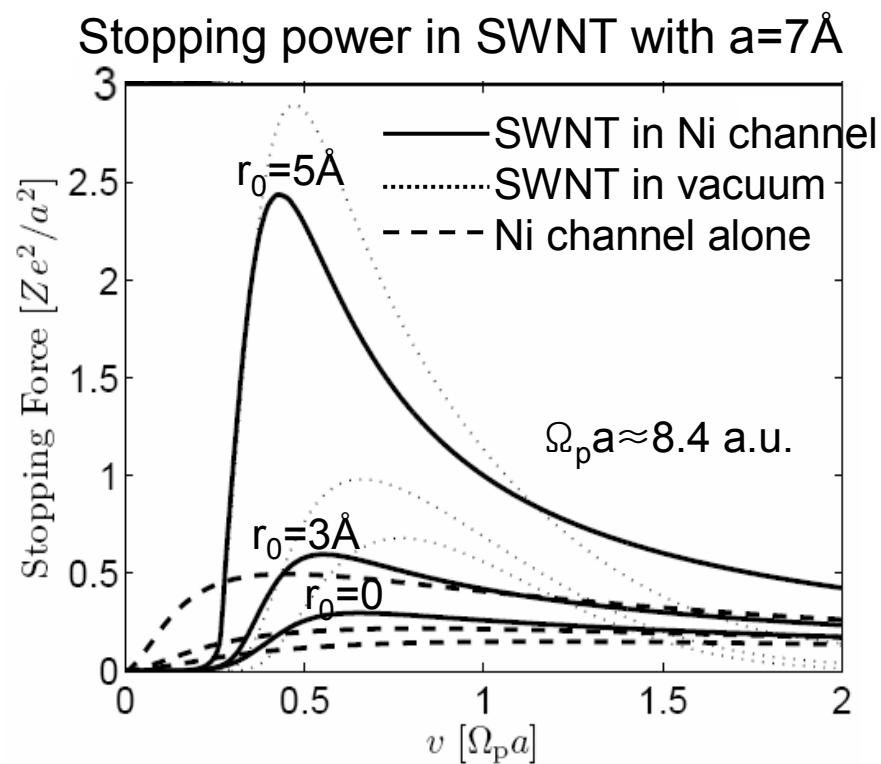
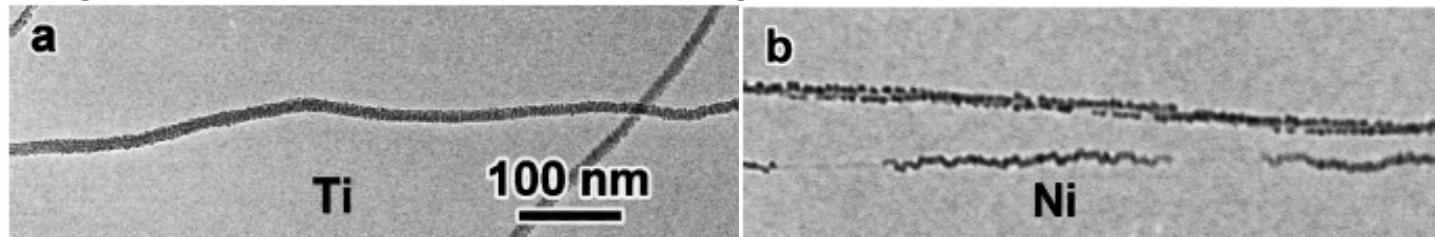
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# Dynamic polarization of SWNT coated by metal

D.J. Mowbray *et al.*, *Phys. Rev. B* (2006) submitted

TEM images of  $a=5$  nm SWNT: Y. Zhang *et al.*, *Chem. Phys. Lett.* 331 (2000) 35

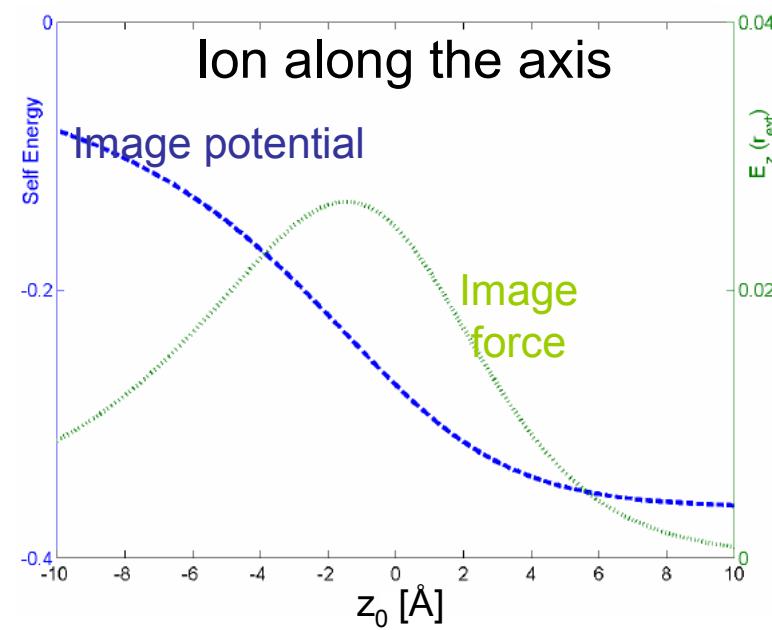
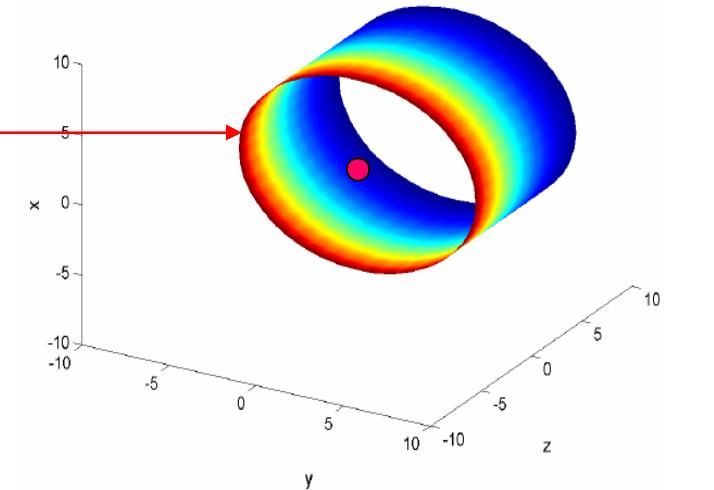
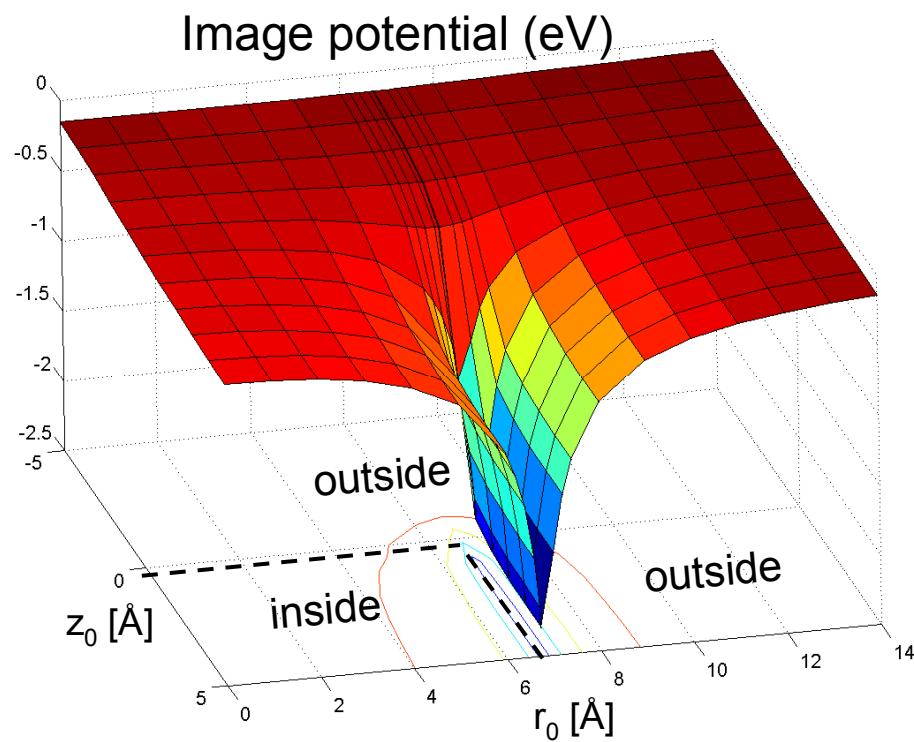


# Static image interaction near an open end of a SWNT

K. Whyte and Z.L. Miskovic, in preparation

Solve integral equation for induced electron density  $n$

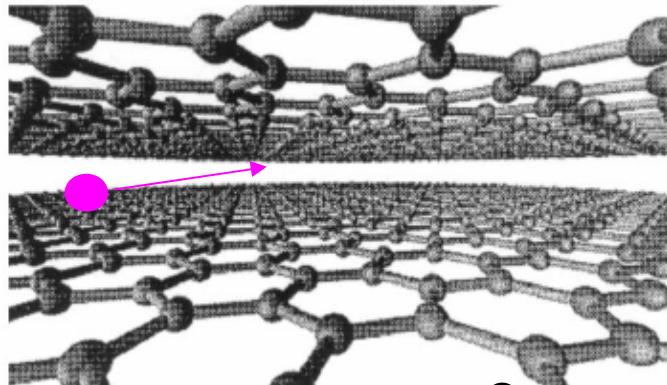
$$\frac{\alpha}{n_0} n(\mathbf{r}) + \iint \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^2\mathbf{r}' = \Phi_{ext}(\mathbf{r})$$



# Planar channeling in Highly Oriented Pyrolytic Graphite

J. Zuloaga *et al.*, ICACS 2006, to be published

Graphene planes in HOPG

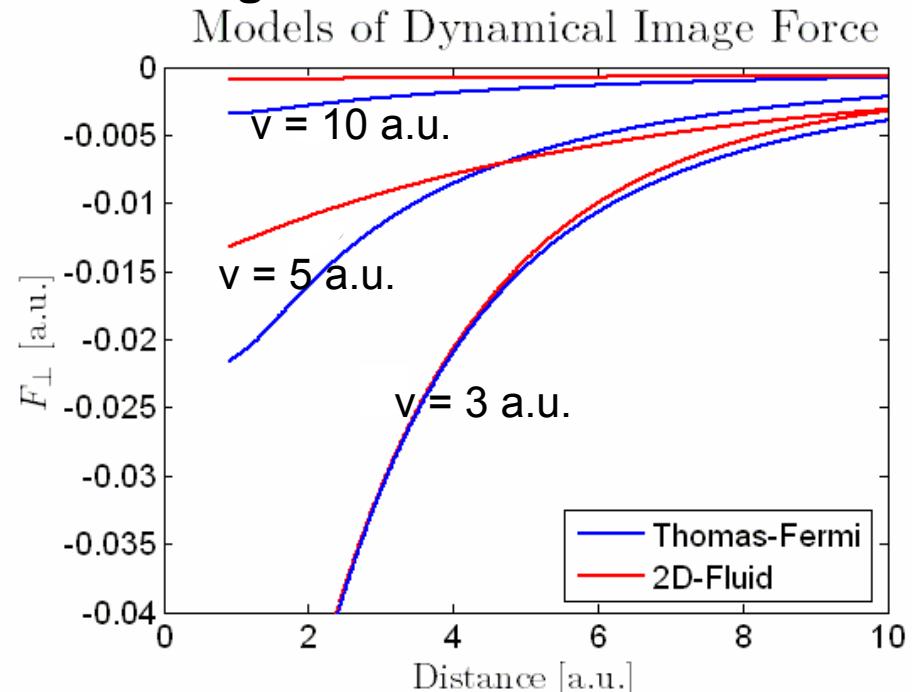
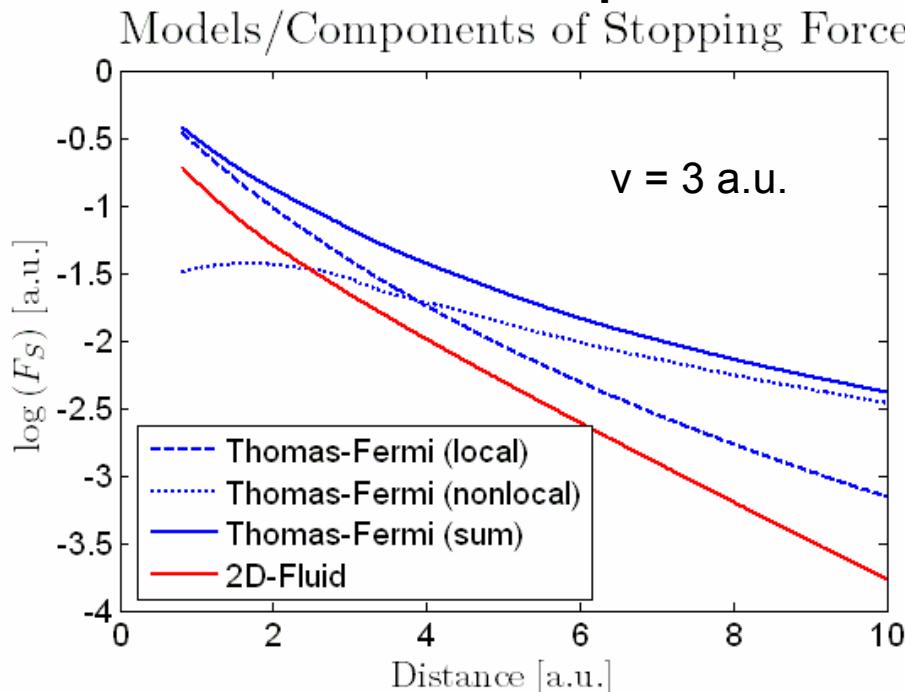


For **single** graphene sheet, calculate stopping power and image force using Kitagawa's dielectric function:

$$\epsilon^{-1}(\mathbf{r}_1, \mathbf{r}_2, \omega) \cong \frac{\omega^2}{\omega^2 - \omega_p^2(\mathbf{r}_1)} \left[ \delta(\mathbf{r}_1 - \mathbf{r}_2) - \frac{1}{\omega^2 - \omega_p^2(\mathbf{r}_2)} \frac{(\mathbf{r}_2 - \mathbf{r}_1) \cdot \vec{\nabla} n(\mathbf{r}_1)}{|\mathbf{r}_2 - \mathbf{r}_1|^3} \right]$$

(High-frequency approx.  $\approx$  Local + Non-local terms)

**Compare 3D and 2D electron-gas models**



# Outline

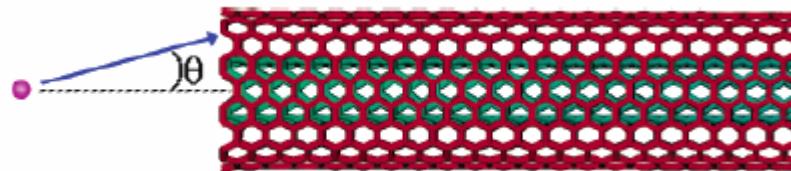
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## Molecular Dynamics (MD) simulations of ion irradiation effects on carbon nanotubes

- Atomistic simulations, solving Newton's equations
- Low impact energies, nuclear stopping dominates
- Empirical potentials (Tersoff/Brenner, van der Waals, and ZBL or Lennard-Jones), truncation issues, no charging
- Ab-initio (DFT) potentials, limited number of C atoms
- Dynamic structure evolution, but limited simulated time
- Finite length of nanotubes (~ 10 nm), energy dissipation
- Simulate temperature effects (annealing of defects)
- Simulate chemical reactions and mechanical response

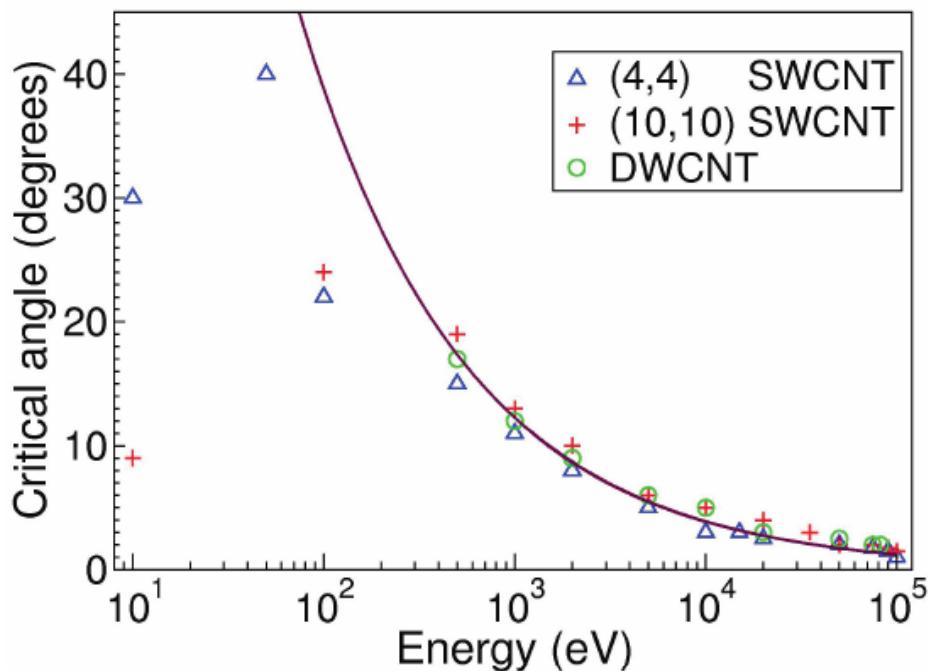
# MD sim. of channelling of C<sup>+</sup> ions in SWNT & DWNT

C.S. Moura and L. Amaral, *J. Phys. Chem. B* 109 (2005) 13515

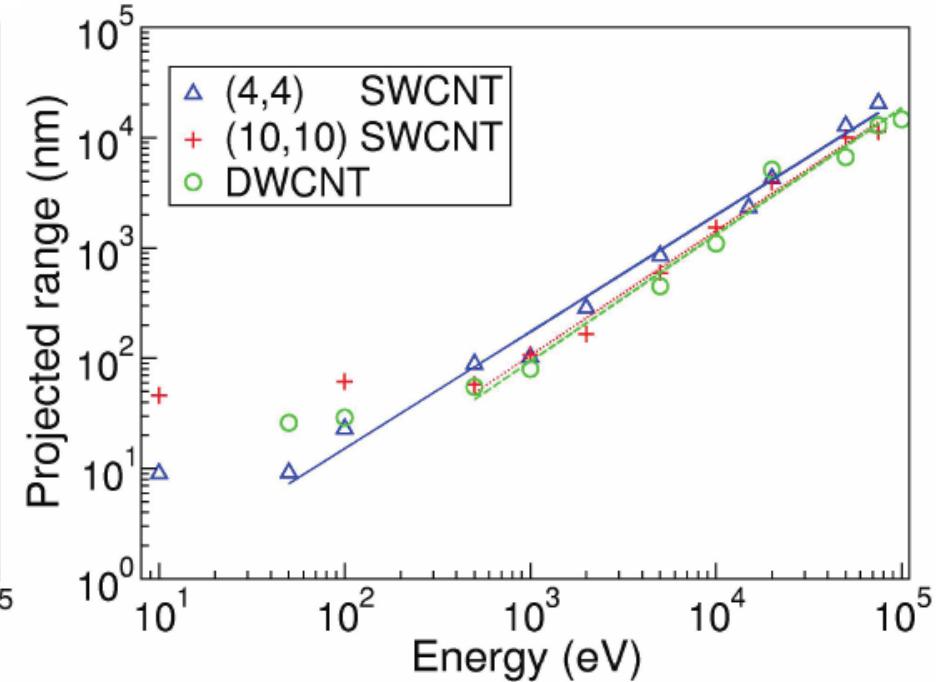


Tersoff potential for C-C in the walls  
ZBL potential for projectile - target

Critical angle vs incident energy

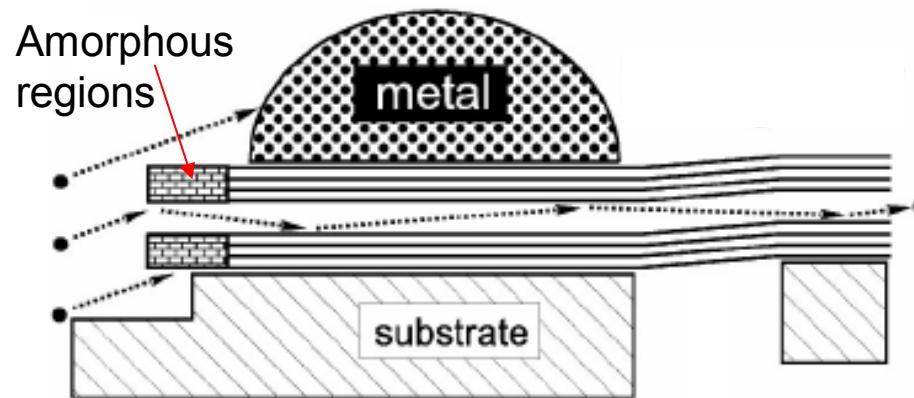


Range vs incident energy



# MD sim. of channelling of keV Ar<sup>+</sup> ions in MWNT

A.V. Krasheninnikov and K. Nordlund., *Phys. Rev. B* 71 (2005) 245408

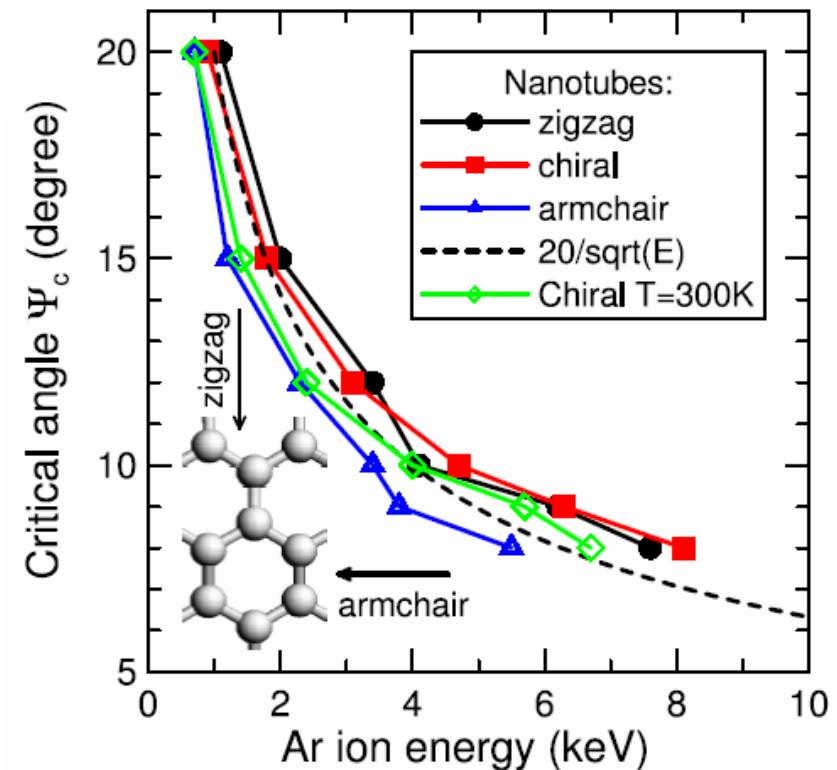


## Conclusions:

- channelling dominated by nuclear energy loss (50-100 eV per collision)
- channelling possible even at low energies and large angles ( $\sim 10^\circ$ )
- less effective between walls of MWNT
- temperature effects weak
- amorphization of entrance opening for high ion beam doses may be problem but central hollow remains open

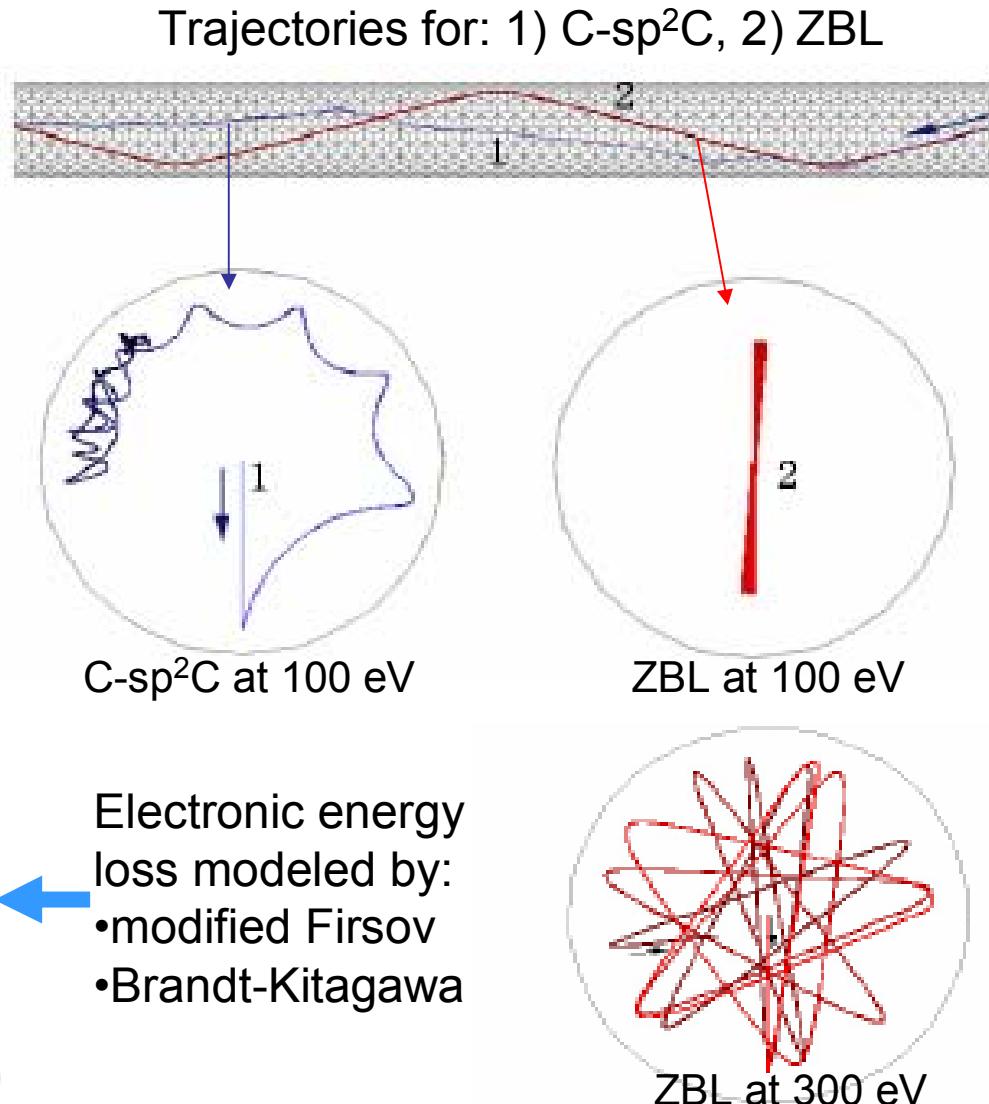
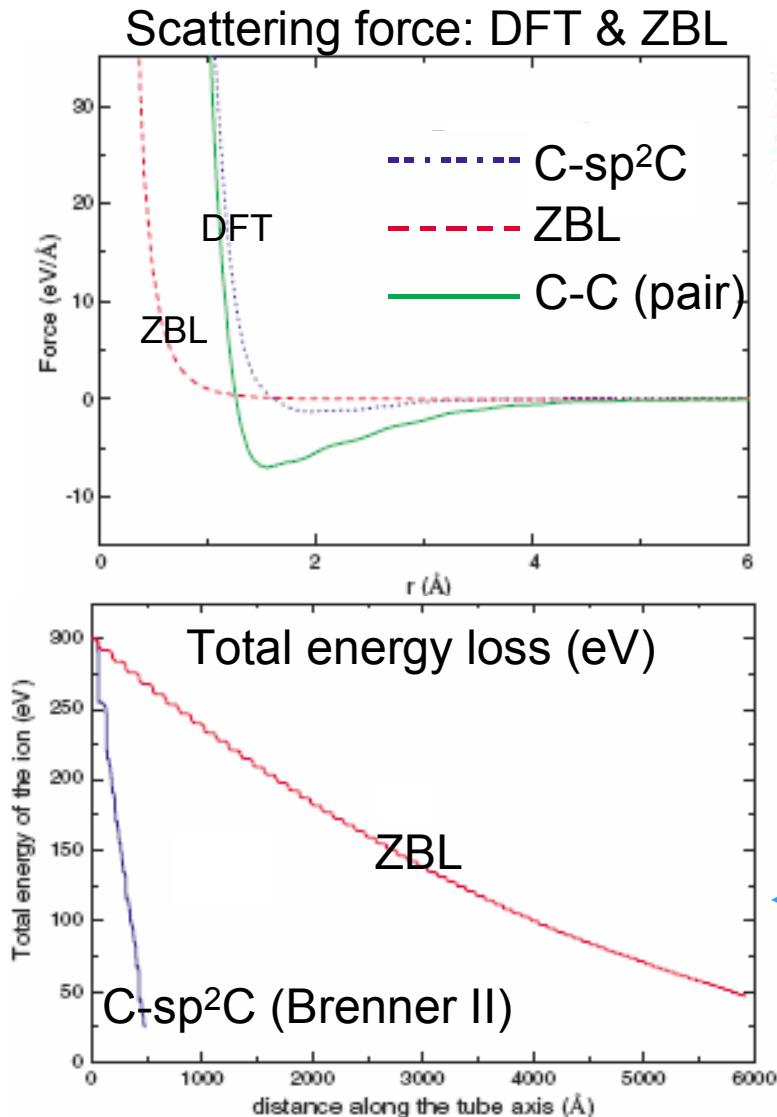
Critical angle for channelling agrees with continuum model

$$\psi_c = \sqrt{U(r_c)/E}$$



# MD sim. of channelling of ~100eV C<sup>+</sup> ions in SWNT

W. Zhang *et al.*, *Nanotechnology* 16 (2005) 2681



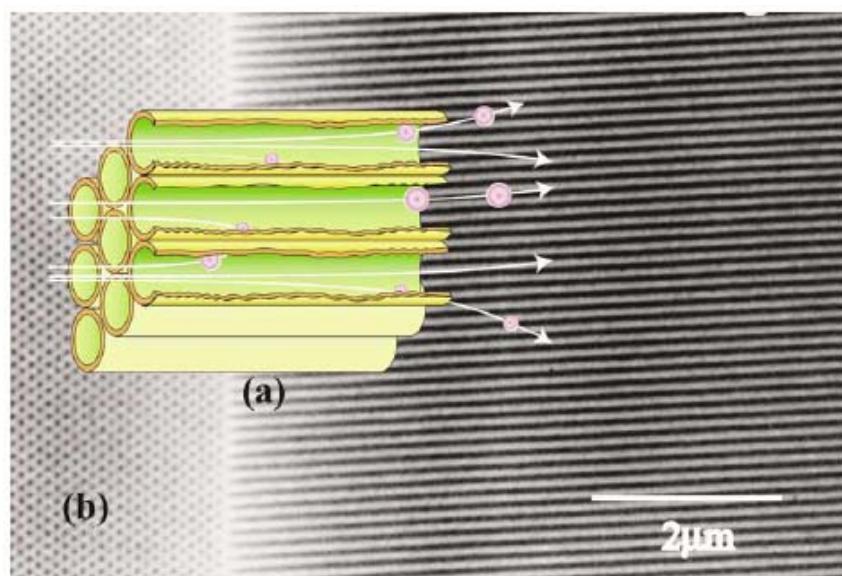
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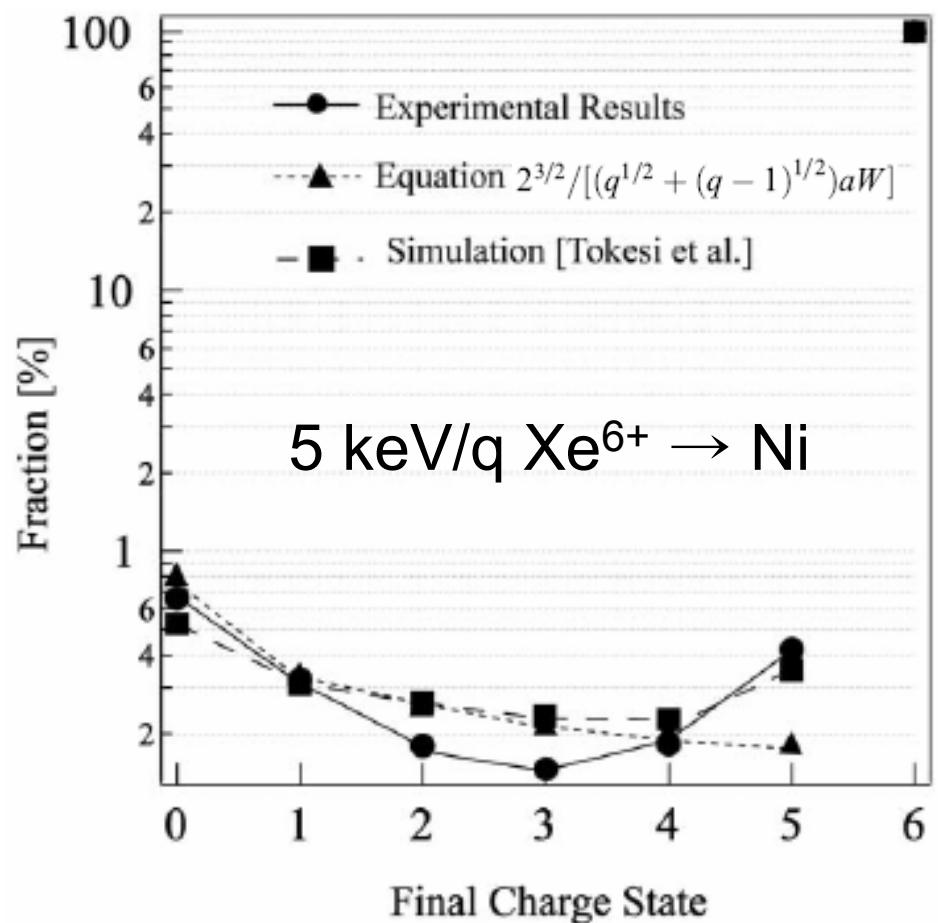
# Transmission of highly-charged ions through arrays of metallic capillaries with diameter $\sim 100$ nm

experiment: Y. Yamazaki, *Nucl. Instr. Meth.* 193 (2002) 516

Schematics of experiment & SEM image of the array



Charge distribution of transmitted ions



# Transmission of highly-charged ions through arrays of metallic capillaries with diameter $\sim 100$ nm

theory: K. Tókési *et al.*, *Phys. Rev. A* 64 (2001) 42902

Use dielectric theory for nano-capillaries to model dynamical image interaction by N.R. Arista, *Phys. Rev. A* 64 (2001) 32901

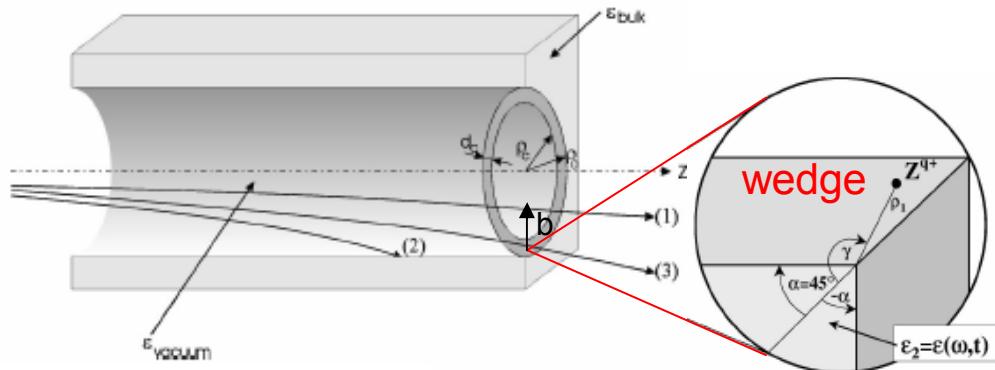
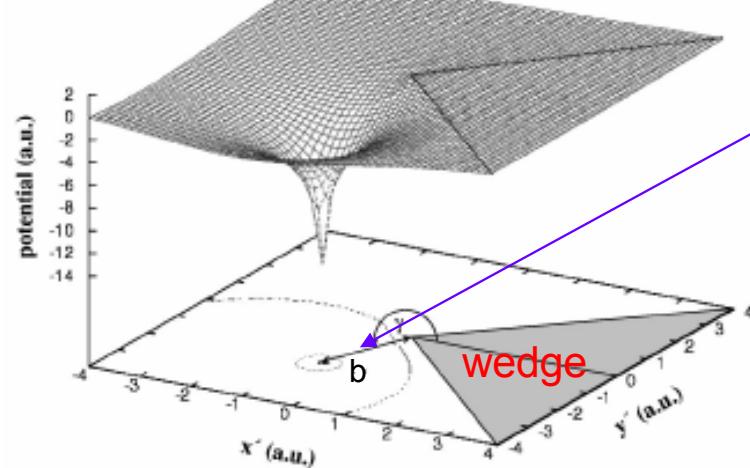
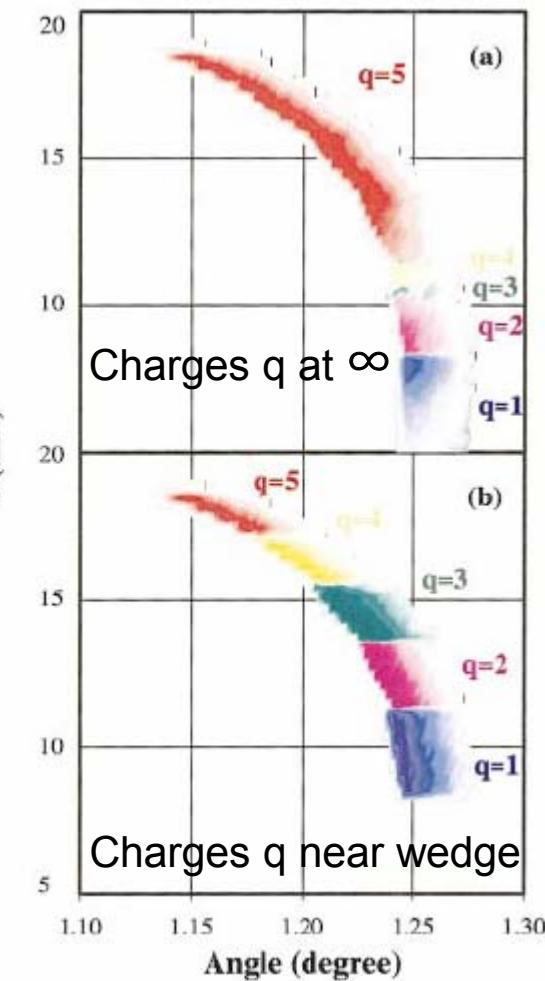


Image potential near the wedge



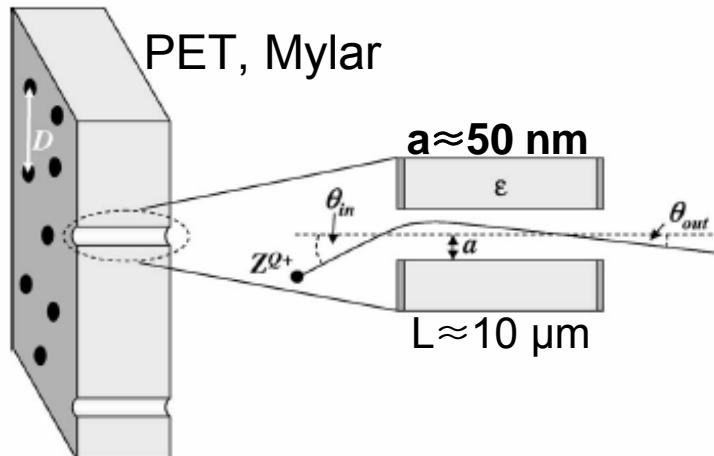
Distributions of 2 keV  $N^{6+} \rightarrow Ni$  vs closest dist.  $b$  and scattering angle



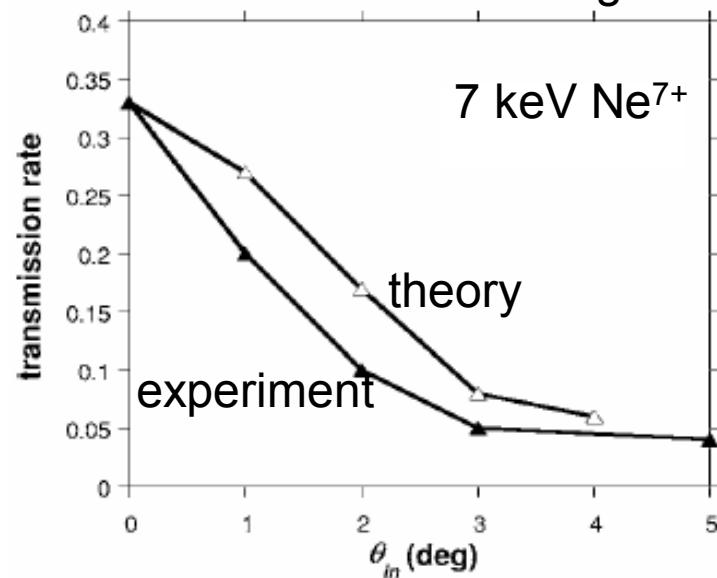
# Guiding keV $\text{Ne}^{7+}$ ions through insulating capillaries

experiment: Gy. Vikor *et al.*, *Nucl. Instr. Meth. B* 233 (2005) 632;

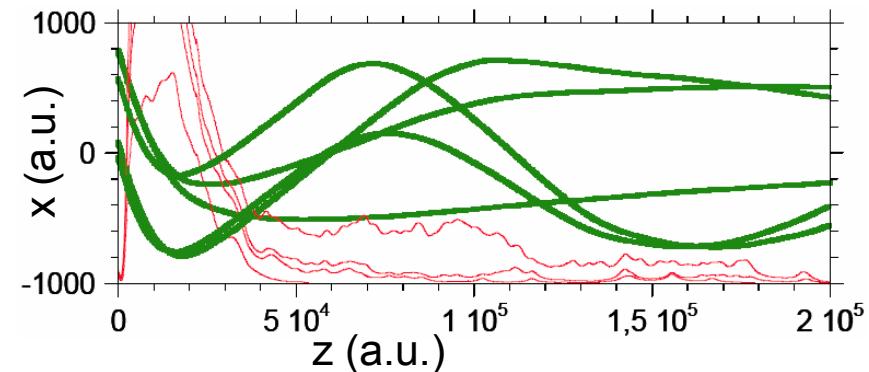
theory: K. Schiessl *et al.*, *Phys. Rev. A* 72 (2005) 62902



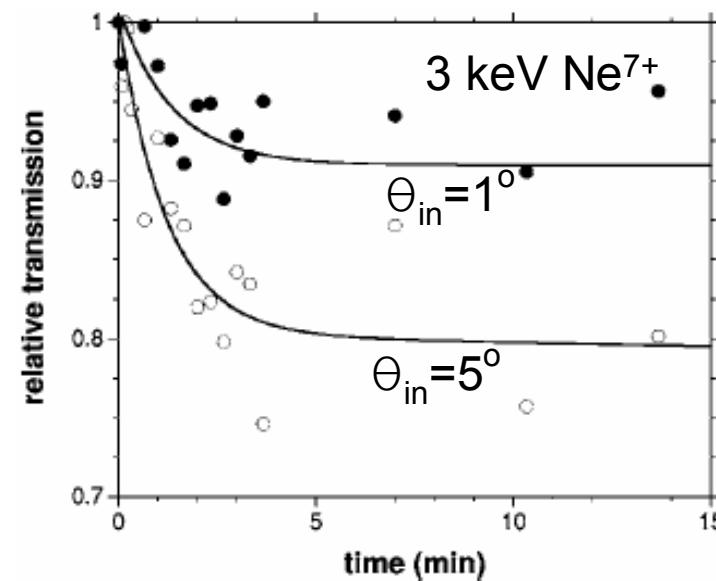
Transmission vs angle



Ion trajectories & deposited charge density



Time dependence of transmission



# Outlook

- Simulations of ion channelling through carbon nanotubes predict great advantages in comparison with single crystals & offer new applications
- Theoretical modeling of ion interactions with nanotubes needs improvements at all energies: ab-initio potentials, dynamic response, energy loss, projectile charge states, entrance effects, defects in nanotube structure, ...
- Experimental realization of ion channelling still pending, but all major technical issues seem manageable (ongoing activity at INFN-LNF & IHEP)
- Exciting new developments expected in near future for particle channeling through carbon nanotubes, following recent success of ion transport through nano-capillaries