Prospects of ion channelling through carbon nanotubes

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Support: NSERC & PREA

Outline

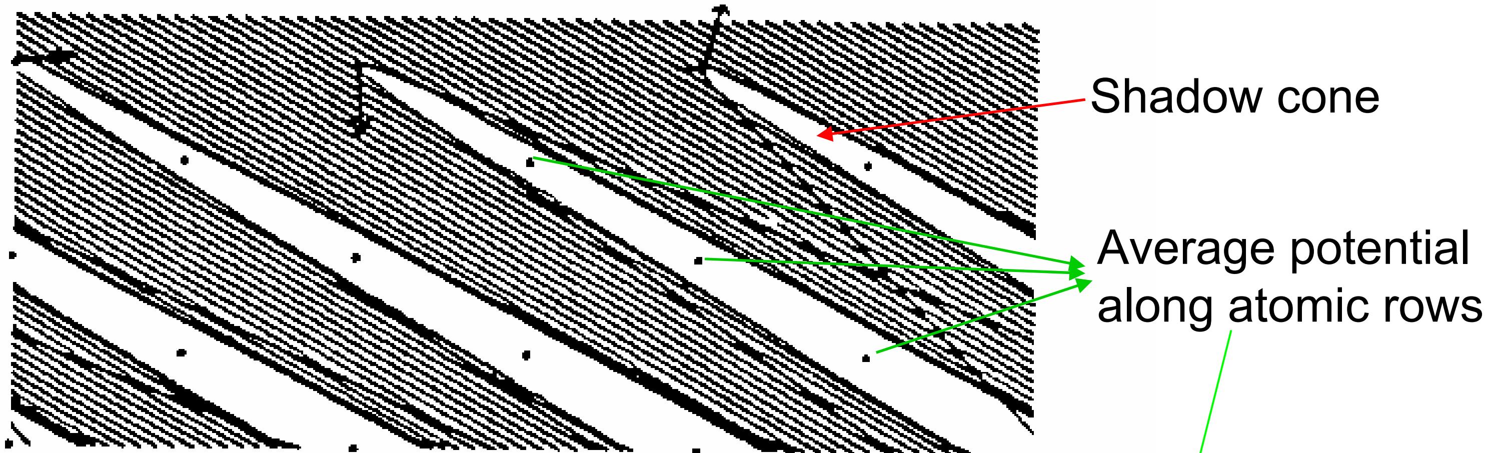
- **Reminder: Channeling in single crystals**
- **Ion interactions with carbon nanotubes**
- **High-energy channeling** (~GeV)
  - Potentials and beam deflection
  - Rainbow effect in short ropes
- **Medium-energy channeling** (~MeV)
  - Modeling the dynamic response
  - Simulations of ion distributions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

Ion channeling in crystals

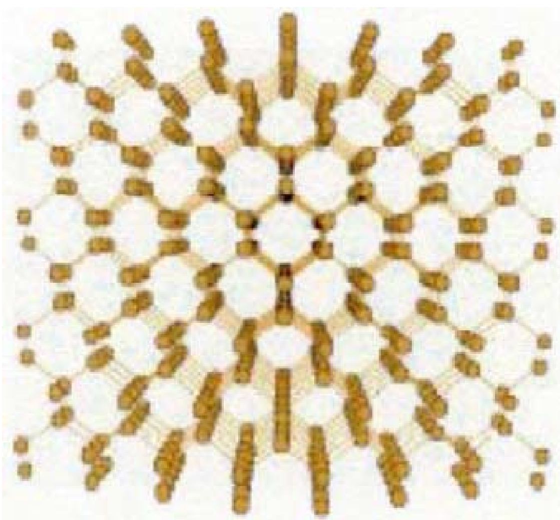
- "Accidental" discovery in computer simulation (1963)
- Theory:
  - Continuum-potential models
  - Binary collision approximation
  - De-channeling, …
- Applications:
  - Medium energies:
    - ion implantation
    - probing impurities in crystals
    - thin films & interface analysis
  - High-energy 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

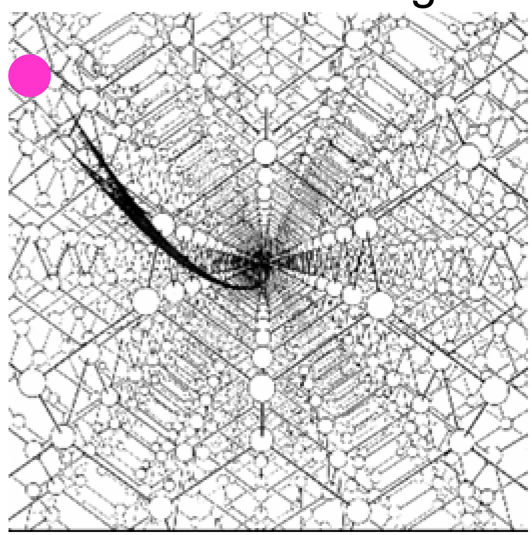
Side view of ion beam channeling



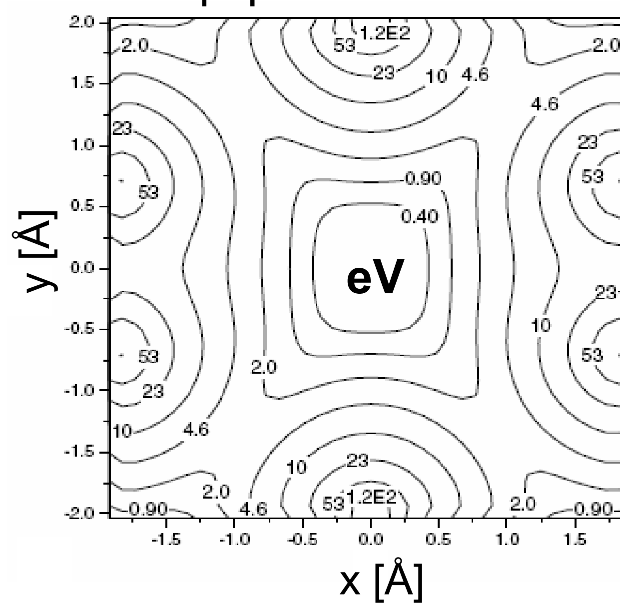
Front view of Si channels



Axial channeling



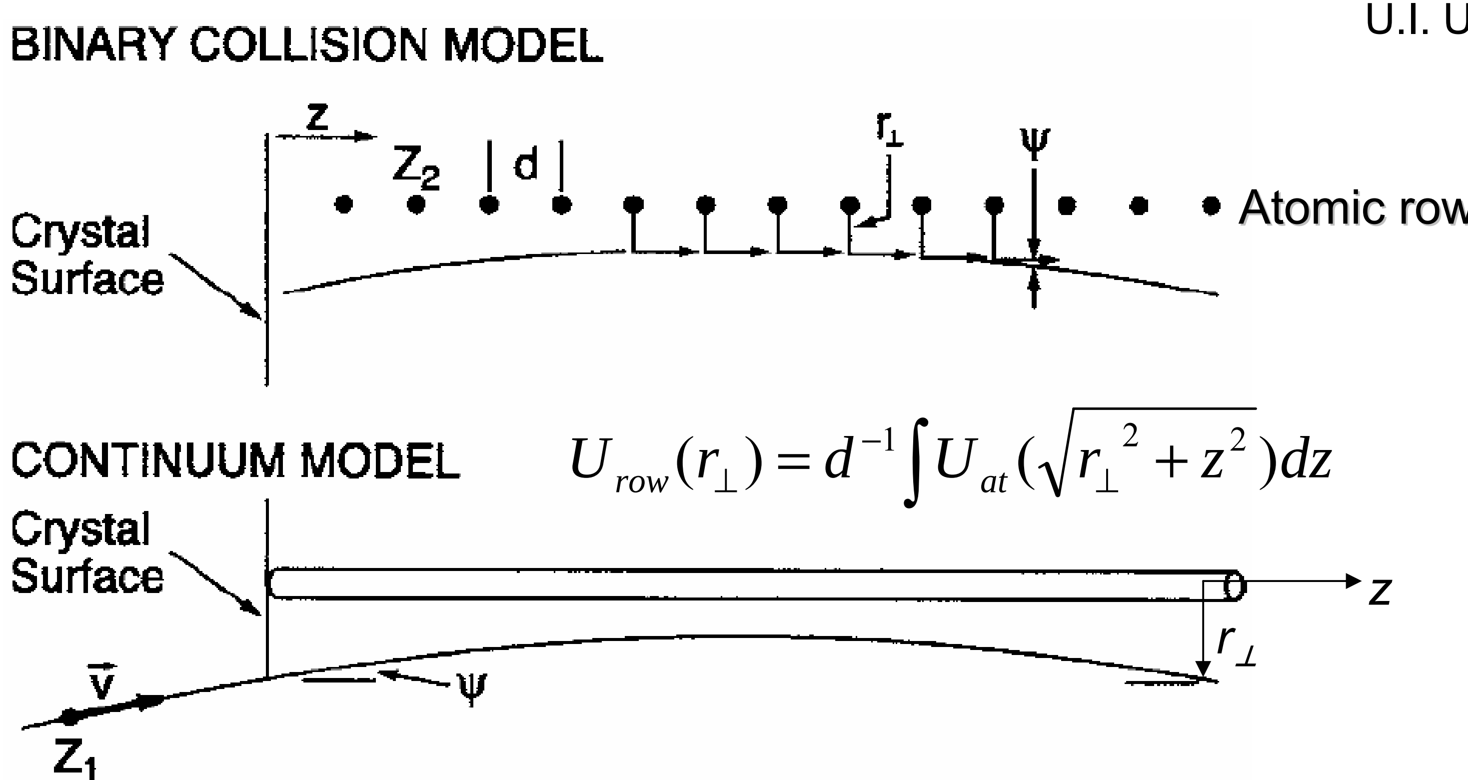
Equipotential curves



Axial channeling through single crystal

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

U.I. Uggerhoj



$$U_{row}(r_\perp) = d^{-1}\int U_{at}(\sqrt{r_\perp^{\,2} + z^2})dz$$

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

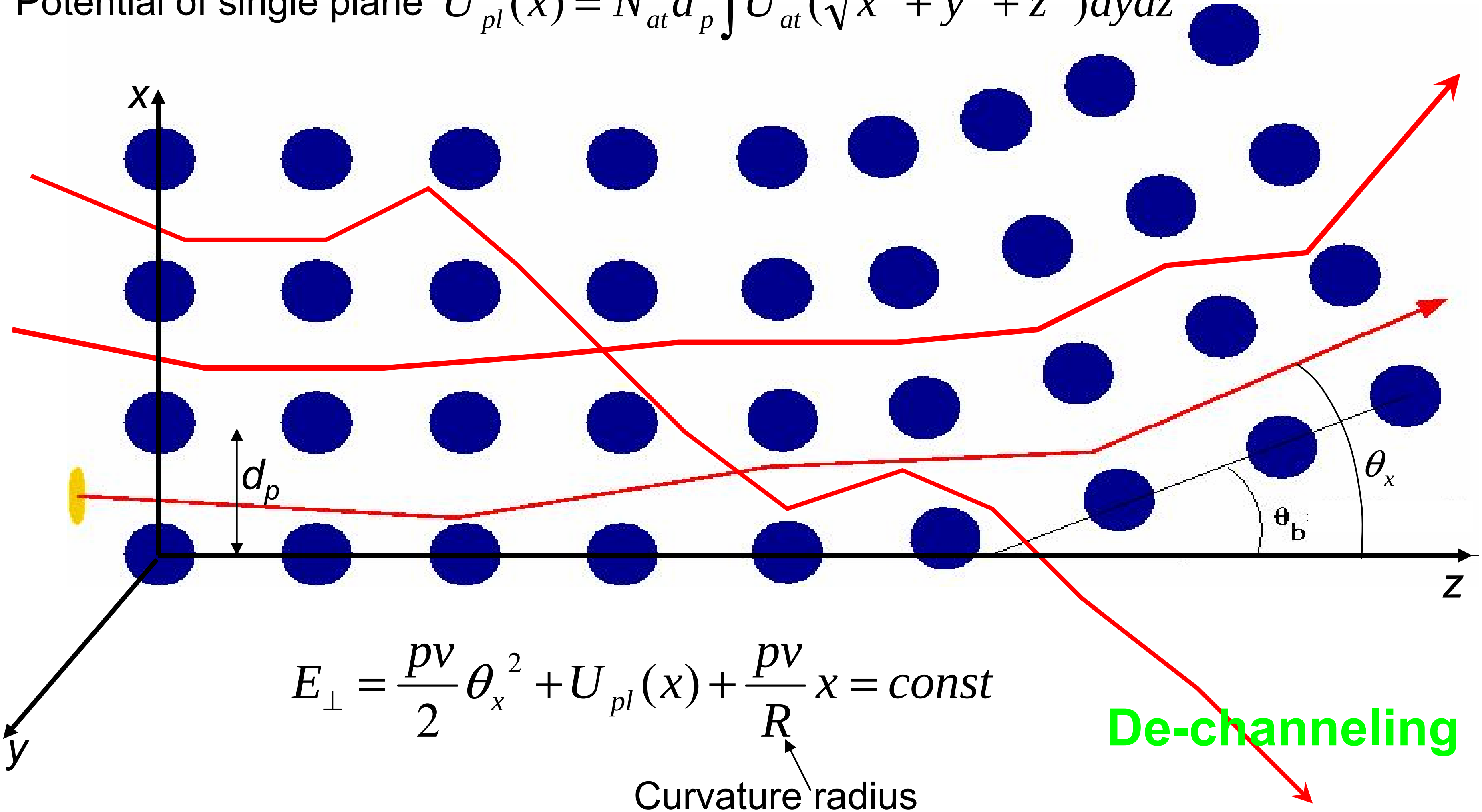
Critical angle for channeling $\psi_c = \sqrt{\frac{4Z_1Z_2e^2}{pvd}}$

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

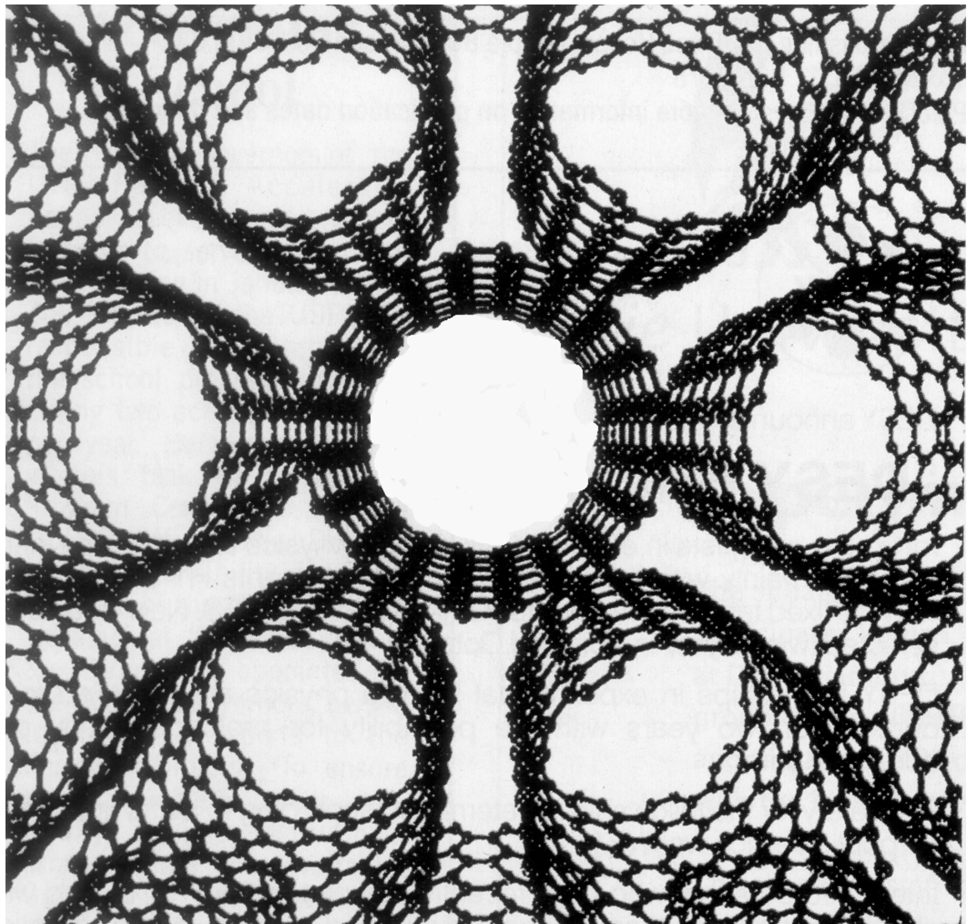
Potential of single plane $U_{pl}(x) = N_{at} d_p \int U_{at}(\sqrt{x^2 + y^2 + z^2}) dydz$



$$E_\perp = \frac{pv}{2}\theta_x^{\ 2} + U_{pl}(x) + \frac{pv}{R} x = const$$

Curvature radius

Ion channeling through carbon nanotubes?
Dream vs. reality



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Carbon nanotubes

❑ Properties:

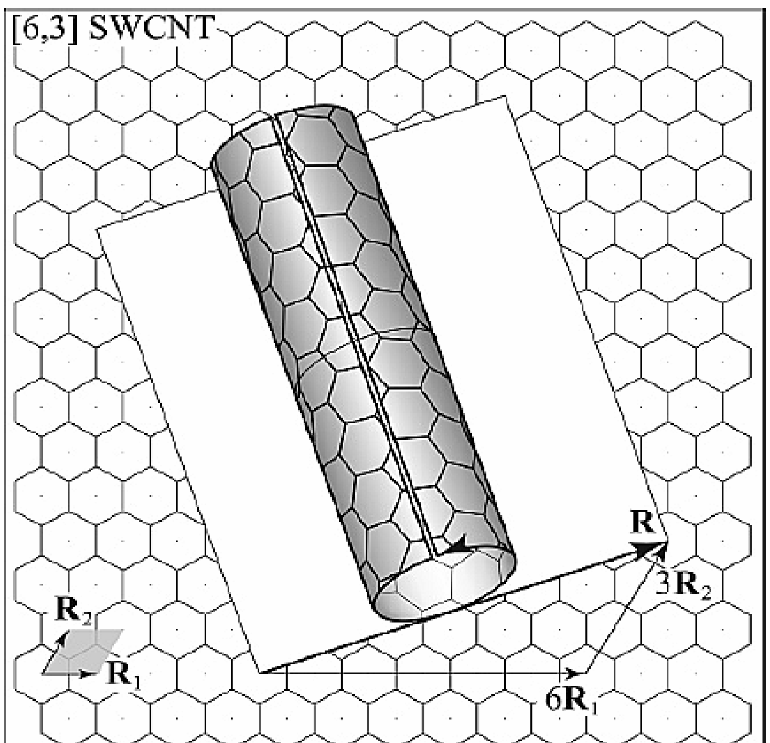
- Electrical, mechanical, thermal
- Dependent on: molecular structure, geometric confinement, local modification

❑ 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)

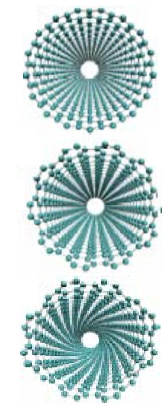
Rolling single graphene sheet:
hexagonal lattice (d=0.14 nm)
of covalently bonded C atoms

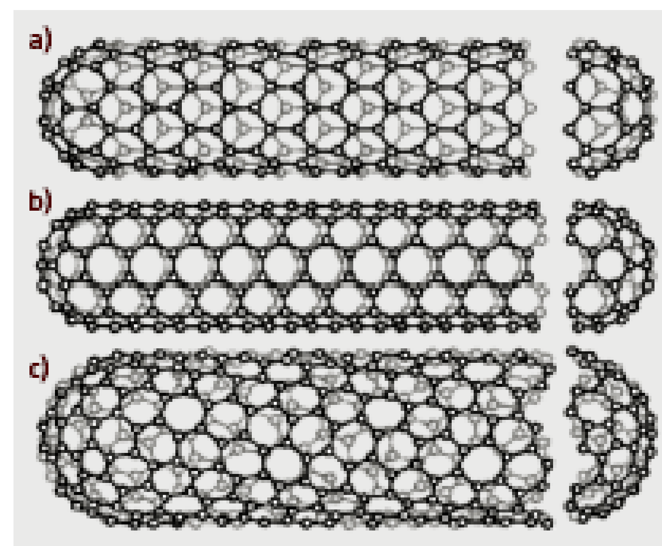


a) zig-zag

b) armchair

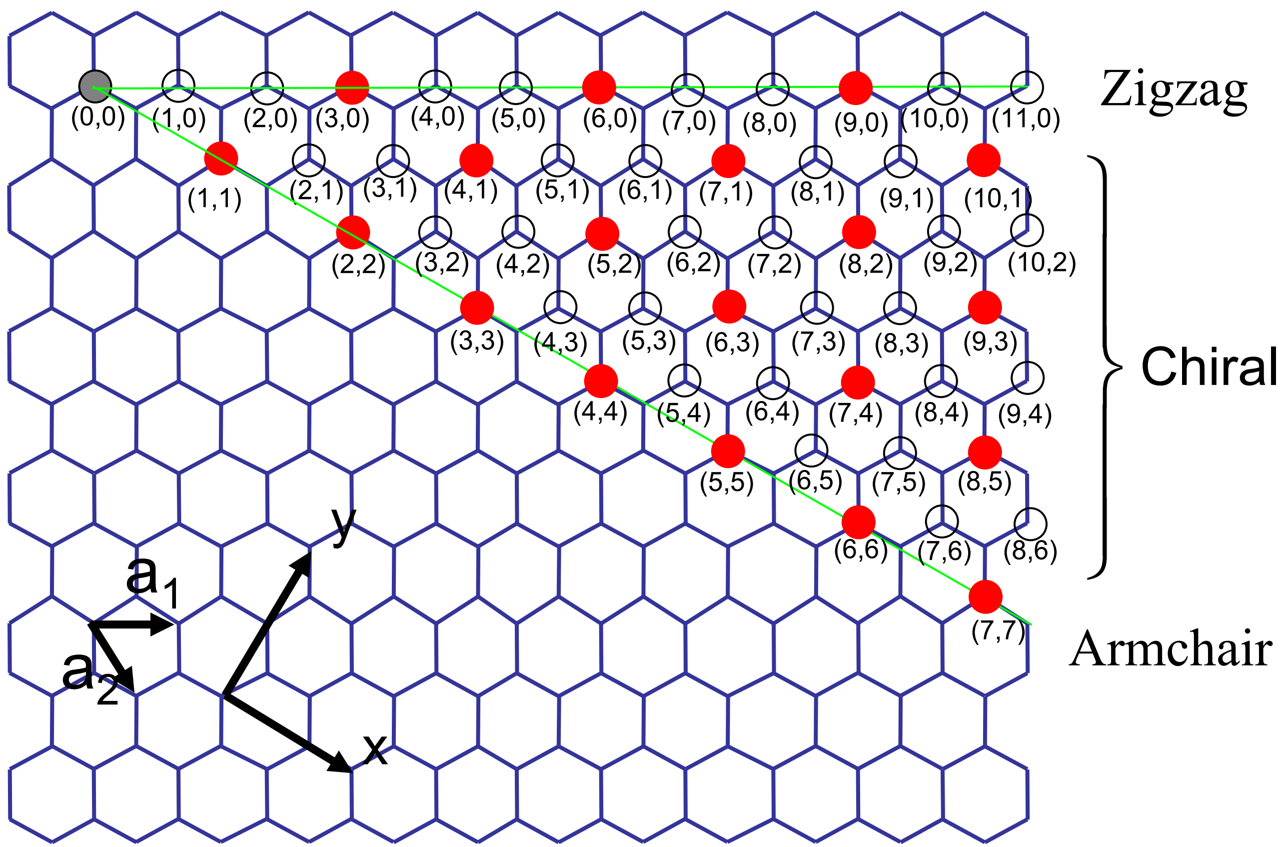
a) chiral





Diameter ~ 1 – 2 nm, Length ~ 1 mm

(n,m) nomenclature of SWNTs

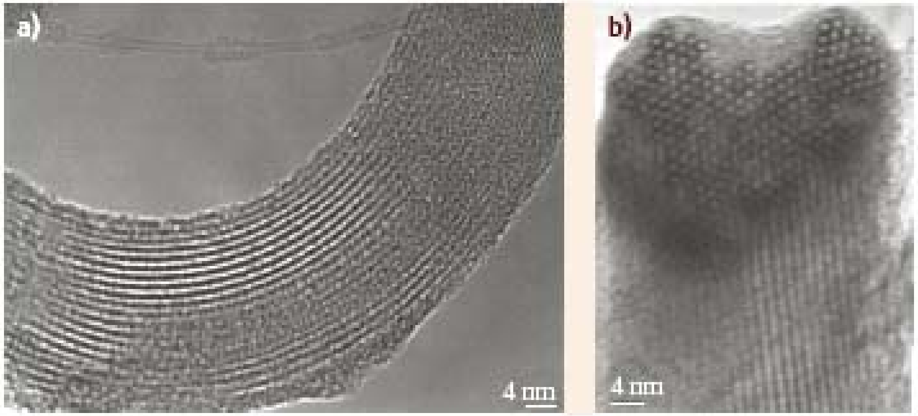


n - m = 3q (q: integer): metallic ●

n - m ≠ 3q (q: integer): semiconductor ○

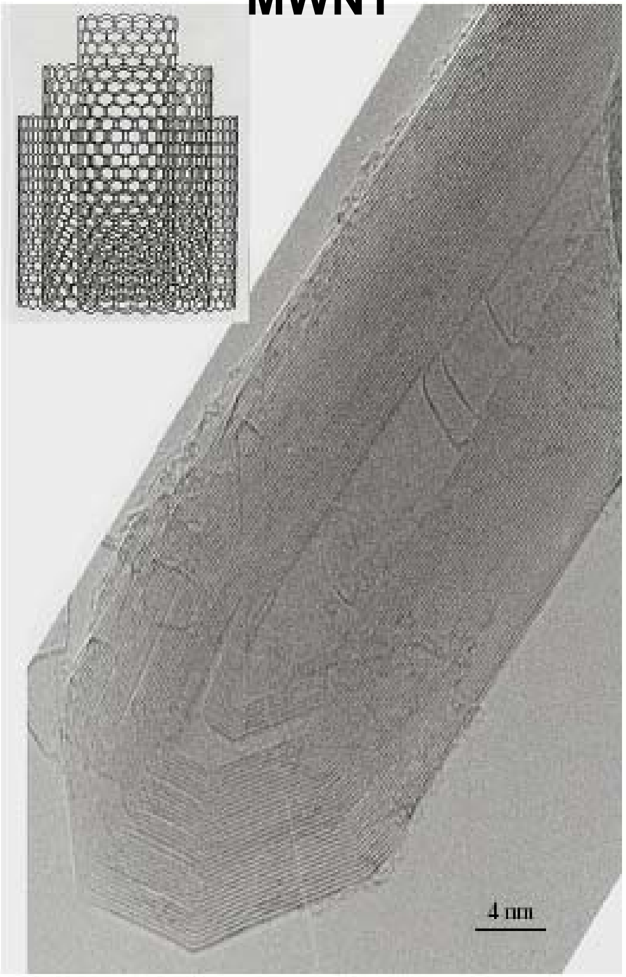
Stacking of nanotubes by van der Waals forces with inter-wall separations ~ 0.34 nm (like in HOPG)

Rope of SWNTs in hexaginal lattice

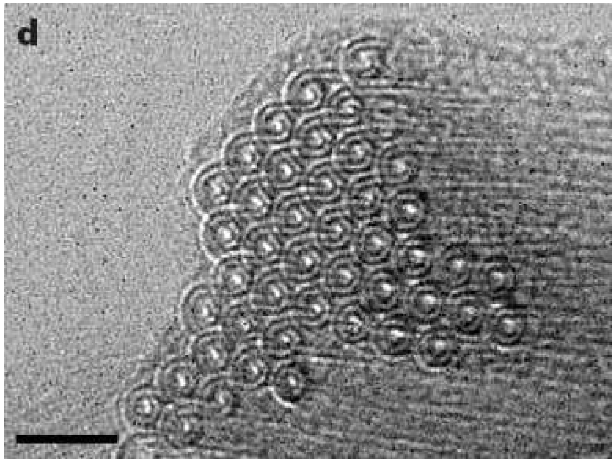


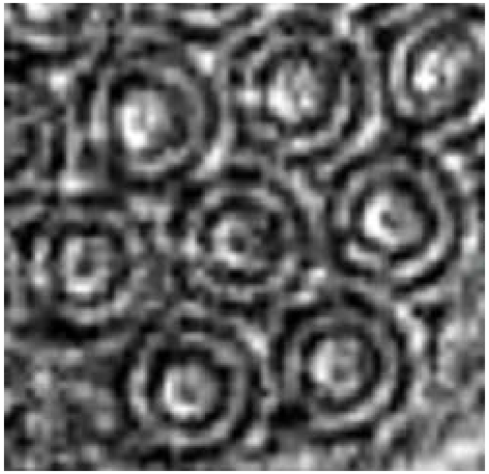
Multi-walled carbon nanotube

MWNT

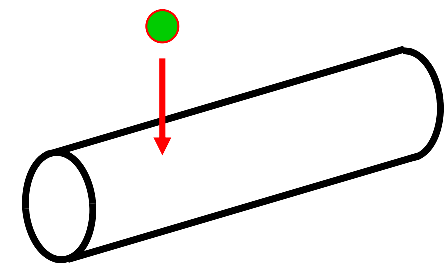


Rope of DWNTs in hexaginal lattice



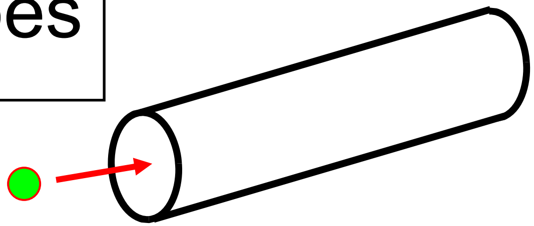


Ion irradiation of carbon nanotubes



- **Beam characteristics:**
  - Directions oblique or perpendicular to nanotube
  - Energies from ~ 100 eV to ~ 100 MeV
  - Heavy and light ions
  - Strong dependence on irradiation dose
  - Beam diameter for local modifications (FIB)
- **Effects on nanotubes:**
  - Creation of local defects (~ 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

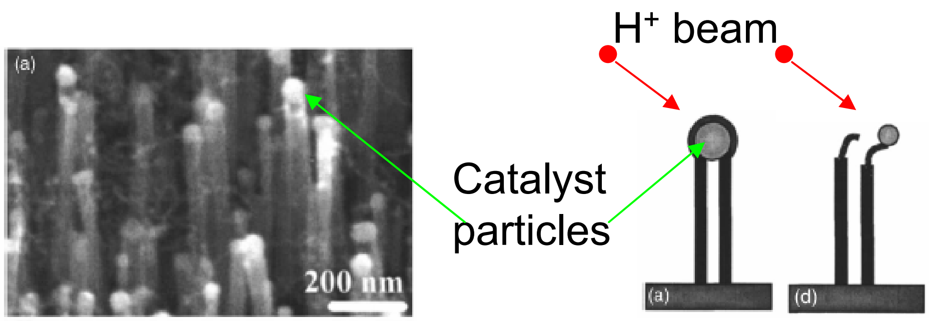


- Advantages over single crystals
  - Wider channels: weaker dechannelling
  - Broader beams (using nanotube ropes)
  - Wider acceptance angles (~ 0.1 rad)
  - Lower minimum ion energies (< 100 eV)
  - 3-D control of beam bending over greater lengths
- Applications
  - Creating and transporting highly 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

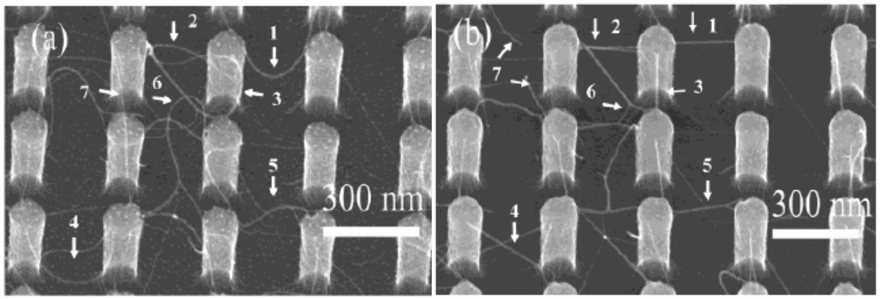
- ❑ **Open ends** (sputter etching)

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



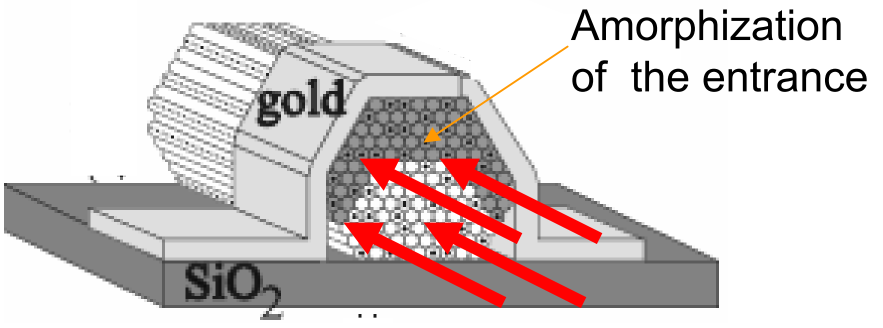
- ❑ **Straightening** (using Ga^+ beam)

  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, $U_{at}(R)$ (Lindhrad, Molière, Doyle-Turner)
- Atomic row potential from longitudinal average

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

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

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

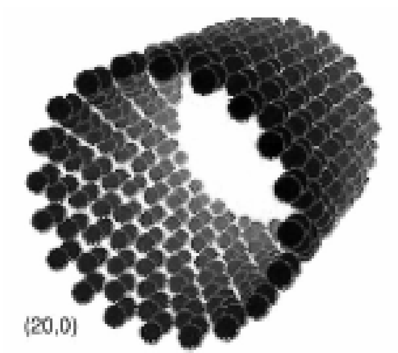
- Wall potential for chiral nanotubes with radius a from averaging over circumference

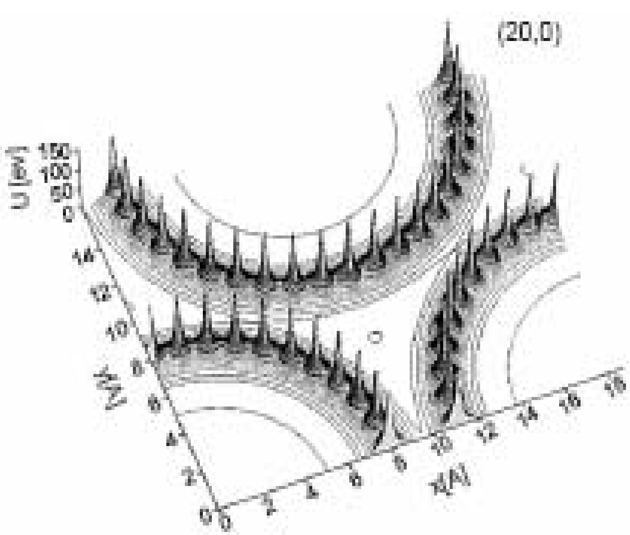
$$U_{chi}(r) = a\sigma_{at} \int_0^{2\pi} \int_{-\infty}^{\infty} U_{at}\left(\sqrt{z^2 + r^2 + a^2 - 2ra\cos\varphi}\right)\, dz\, d\varphi$$

Continuum approximations for the repulsive atomic potential in SWNTs

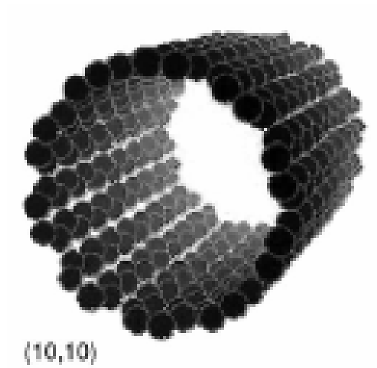
X. Artru *et al.*, *Phys. Reports* 412 (2005) 89

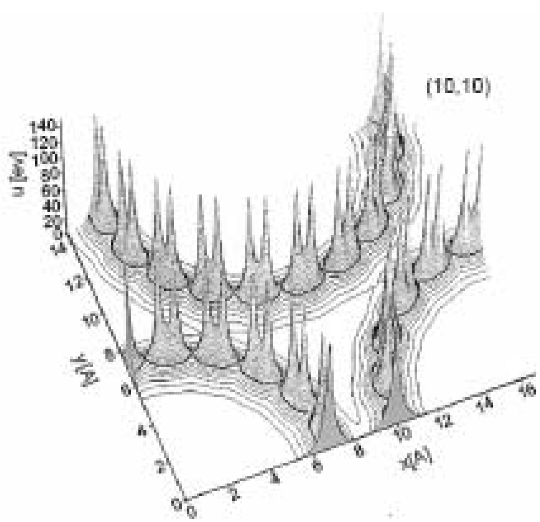
Zig-zag



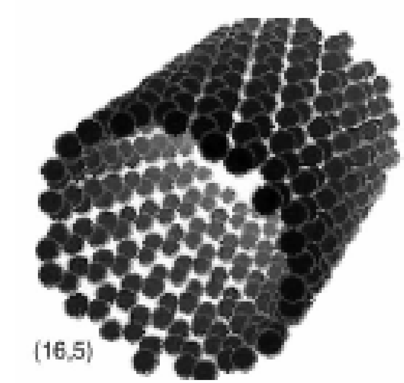


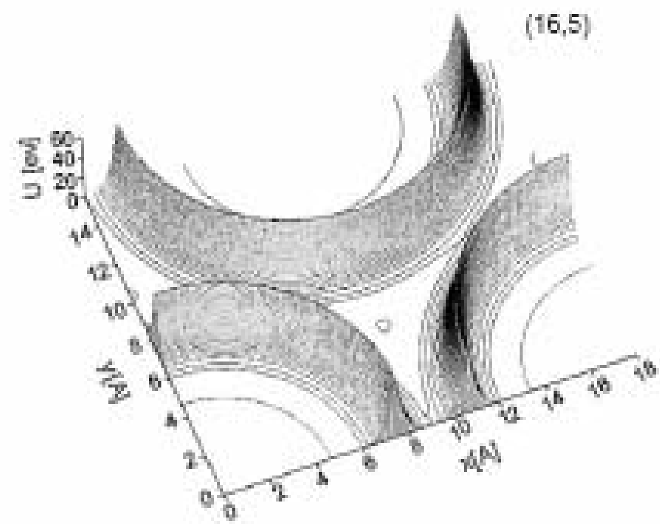
Armchair





Chiral

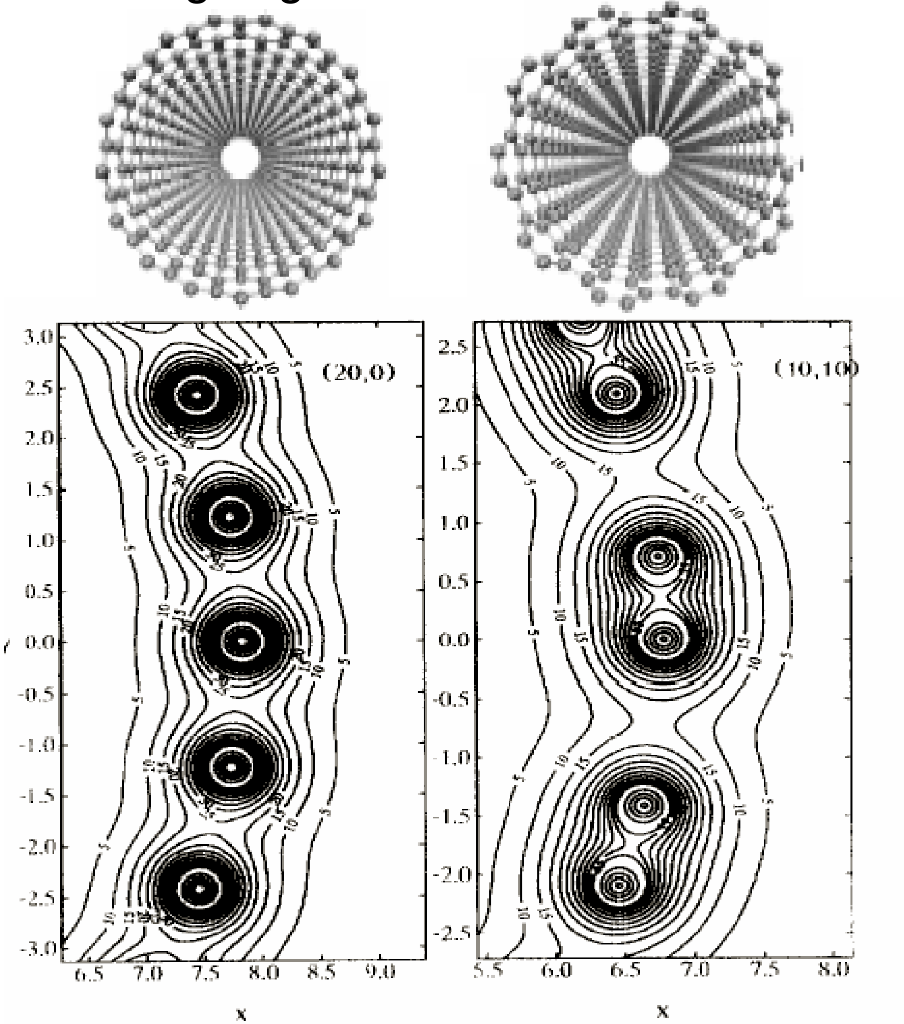




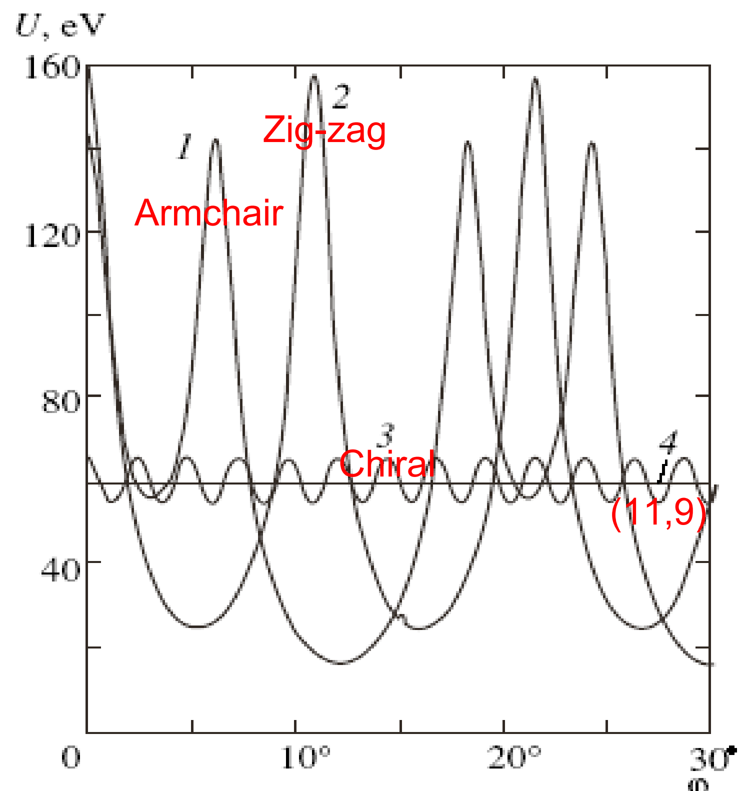
Continuum potential due to atomic rows in achiral SWNTs

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

Zig-zag　　Armchair

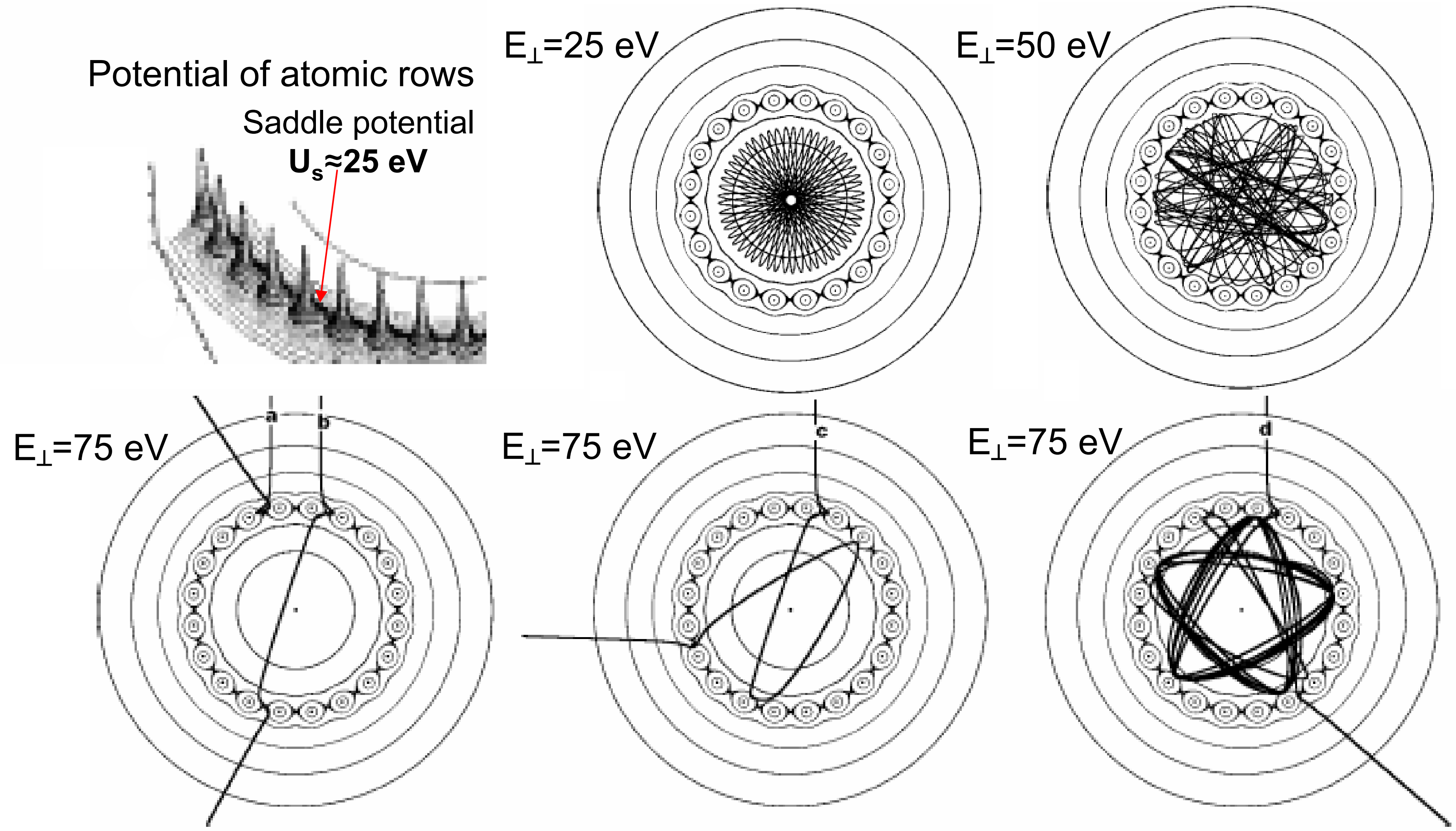


Angular variation of potential barrier at the nanotube wall



Trajectories for ion channeling in a zig-zag SWNT(10,0) at several transverse energies $E_\perp$ relative to saddle U_s

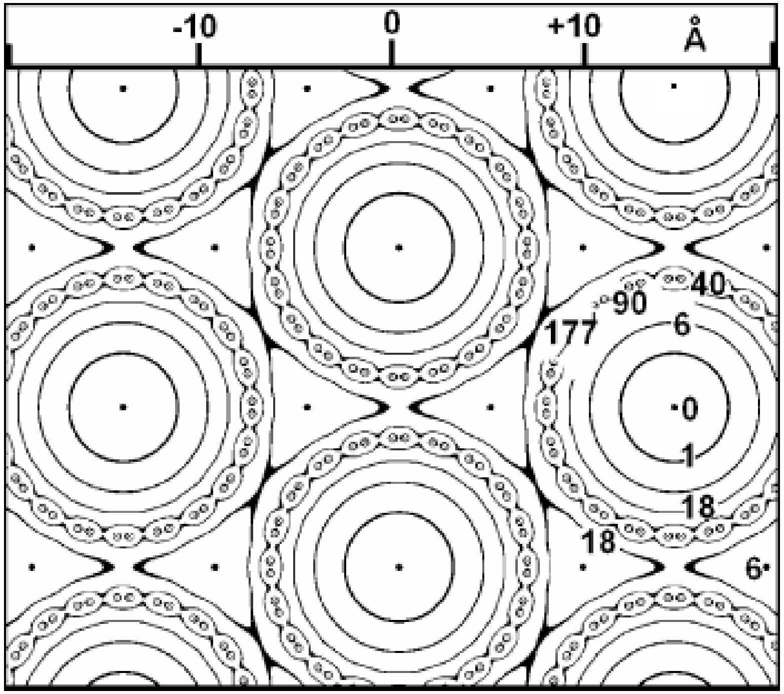
X. Artru *et al., Phys. Reports* 412 (2005) 89



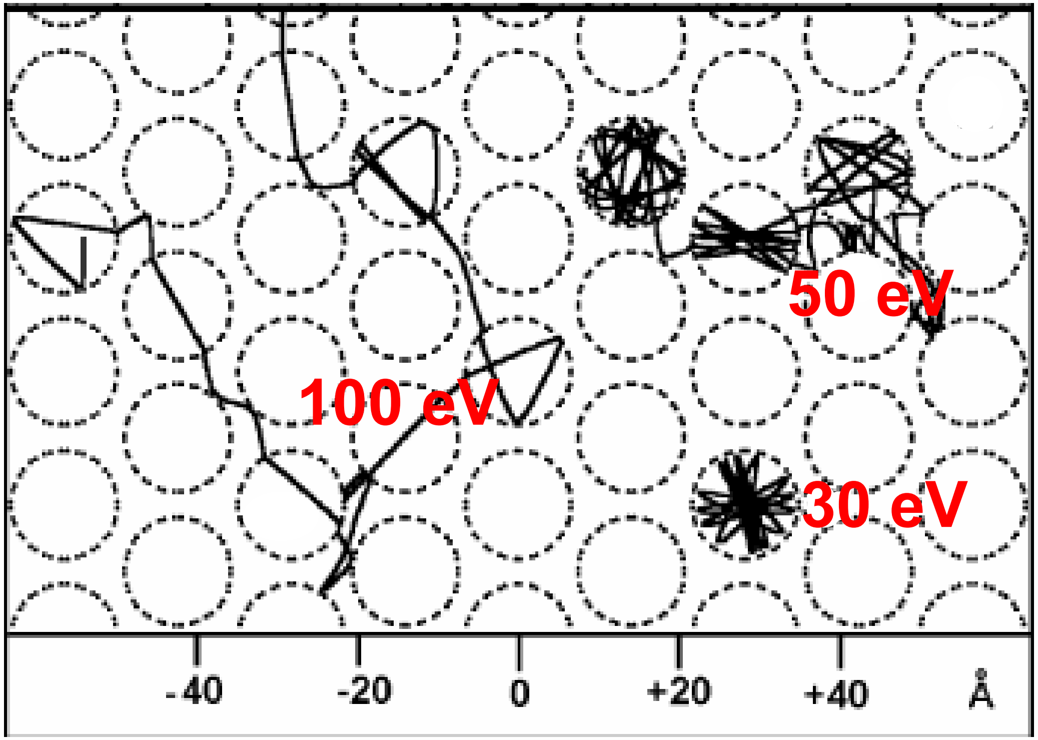
Ion channelling through <u>rope</u> of <u>armchair</u> SWNTs(10,10)

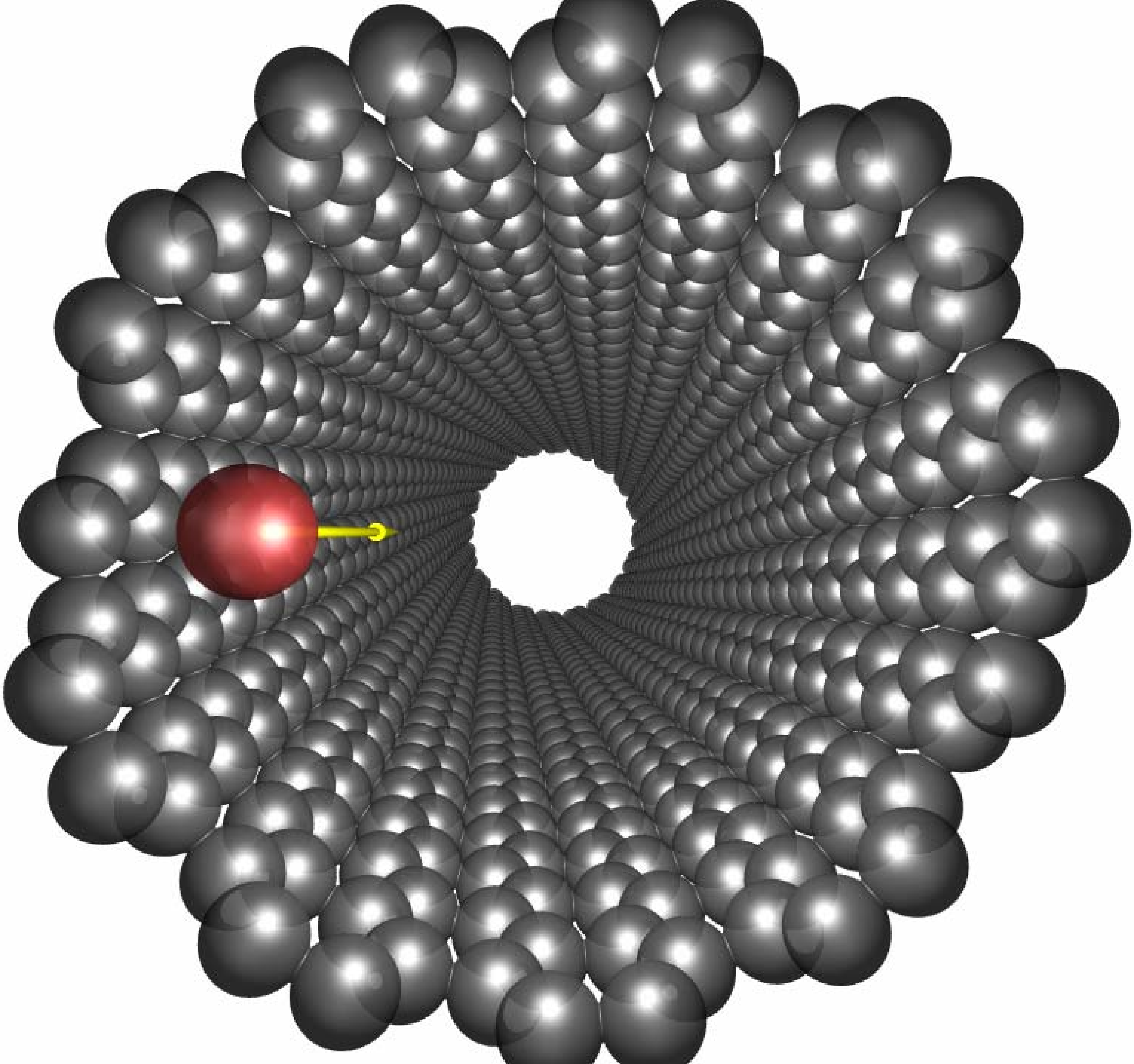
A.A. Greenenko and N.F. Shulga, *Nucl. Instr. Meth.* B 205 (2003) 767

Equi-potential surfaces (eV)



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

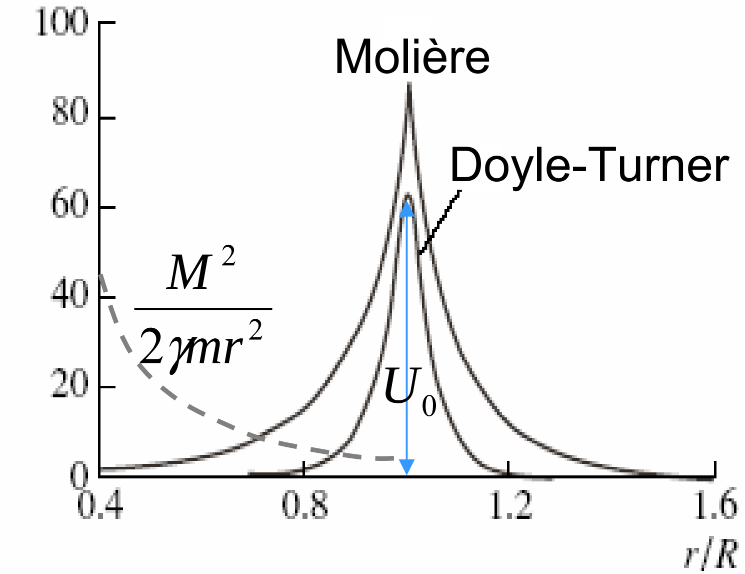




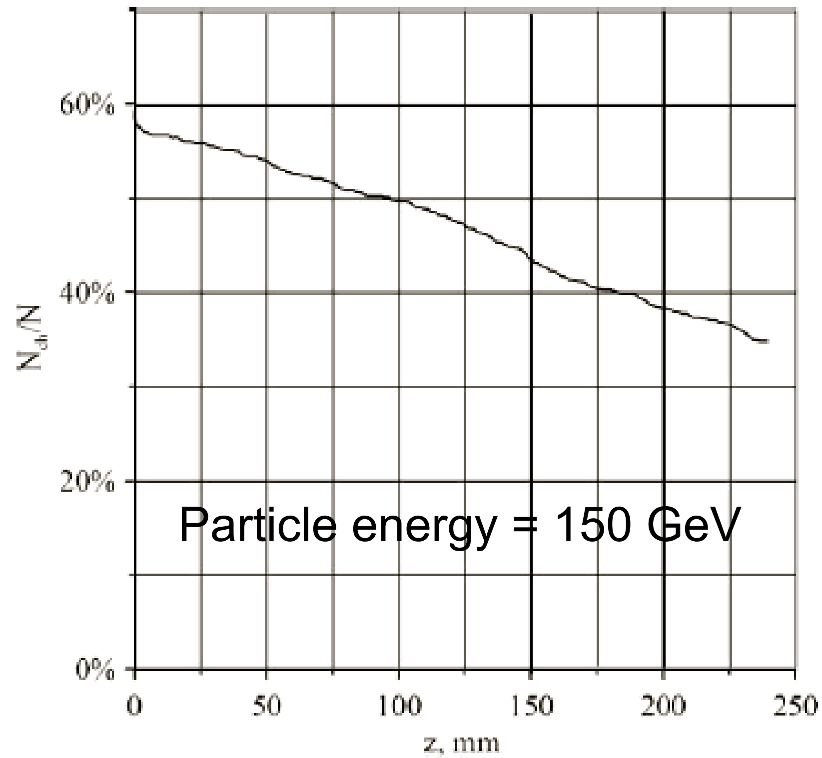
Ion channelling through a straight chiral SWNT(11,9)

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

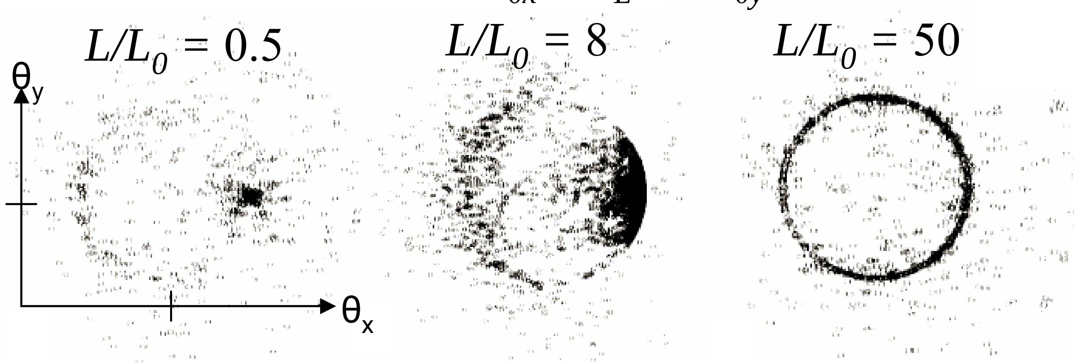
Axially symmetric potential



Removal of ions due to dechanneling



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



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

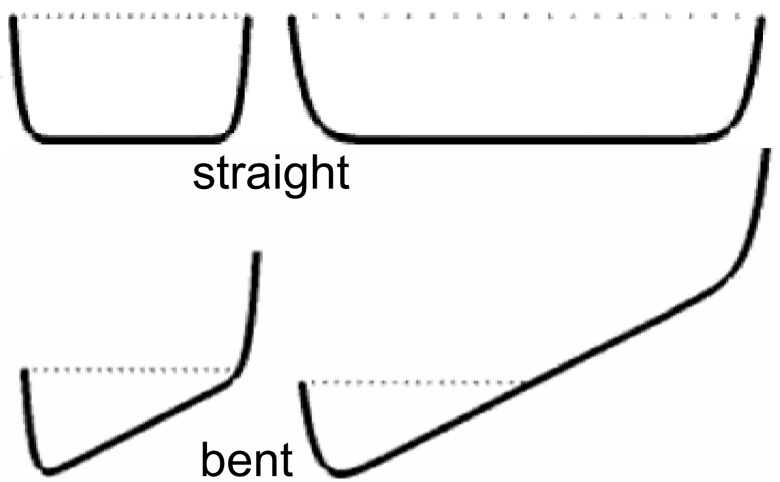
$$L_0 \equiv d / 2\theta_L$$

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

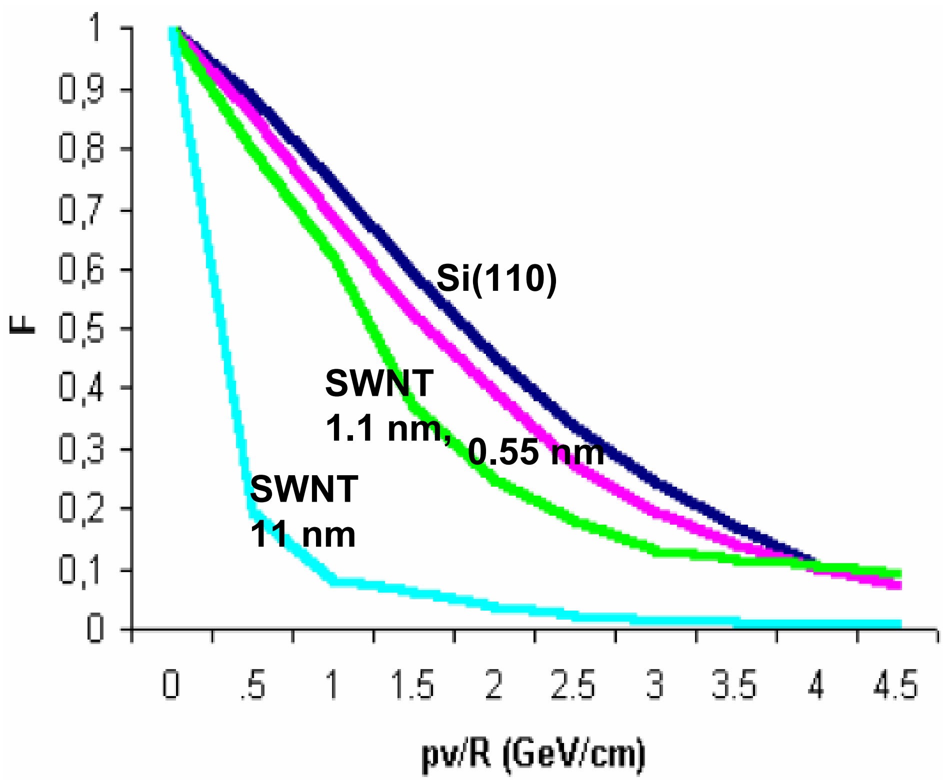
V.M. Biryukov and S. Bellucci, *Phys. Lett.* B 542 (2002) 111

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

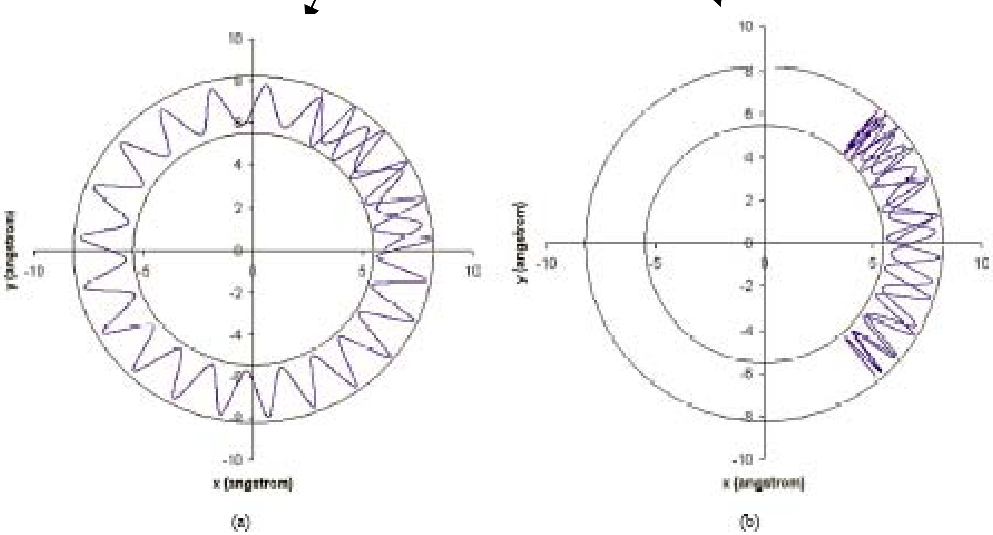


Conclusion: wide SWNTs are not more effective for beam steering

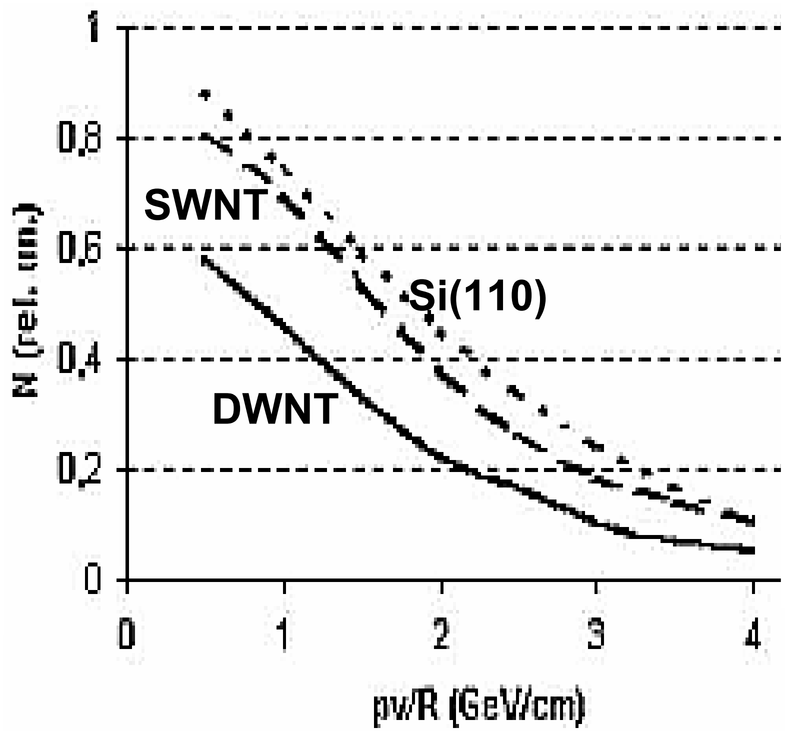
GeV proton beam steering in bent <u>chiral</u> DWNTs

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

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

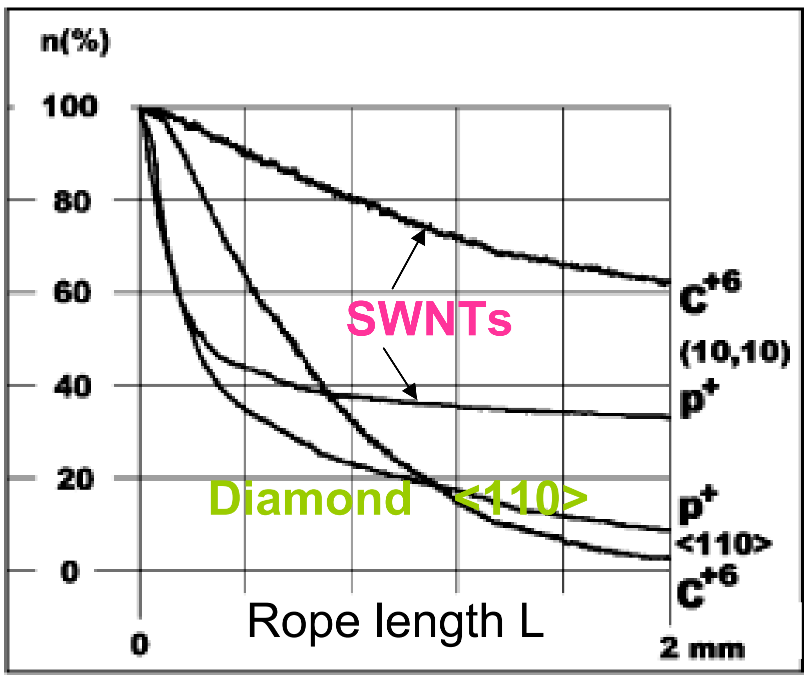


Fractions of protons channelled through: Si(110) crystal channel, SWNT with diameter 0.55 nm, and between walls of a DWNT



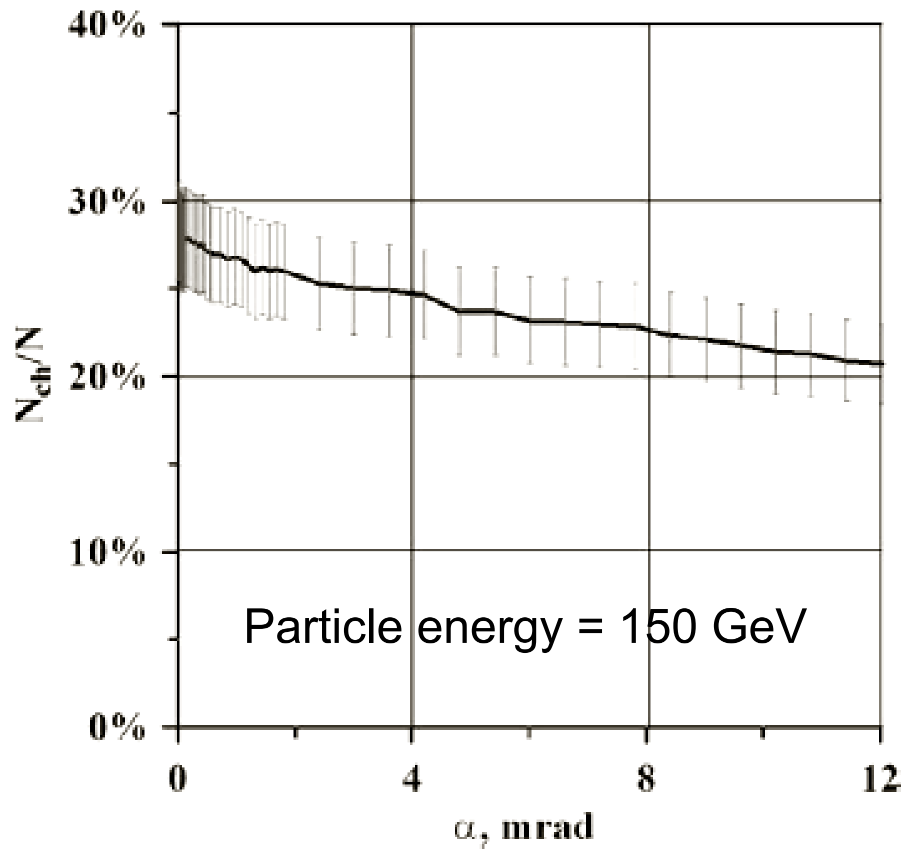
Deflected beam fractions in bent ropes of SWNTs

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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Canadian Rockies, Banff National Park, Alberta

Theory of rainbows in <u>short</u> 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 is

$$\sigma \approx 1/|J|$$

- $J = \partial_x \Theta_x \partial_y \Theta_y - \partial_x \Theta_y \partial_y \Theta_x$ 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

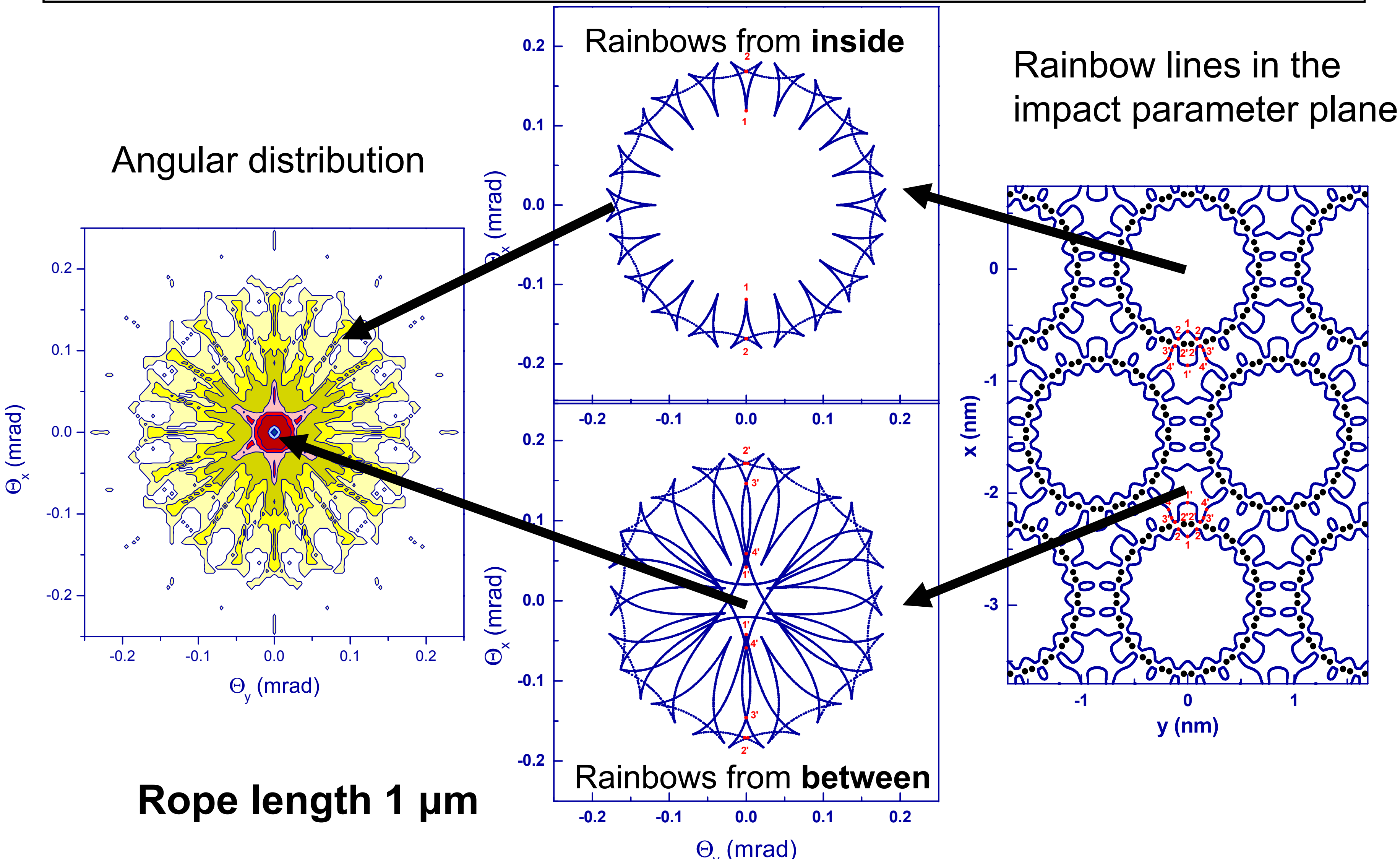
$$J(x_0, y_0 ; L) = 0$$

- Total potential is sum over all atomic rows on all nanotubes in the rope

- Could be used for precise measurements of the interaction potentials and thus of the electron density in carbon nanotubes

Rainbow effect after 1GeV proton channelling through a <u>short</u> rope of <u>armchair</u> SWNTs(10,10)

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

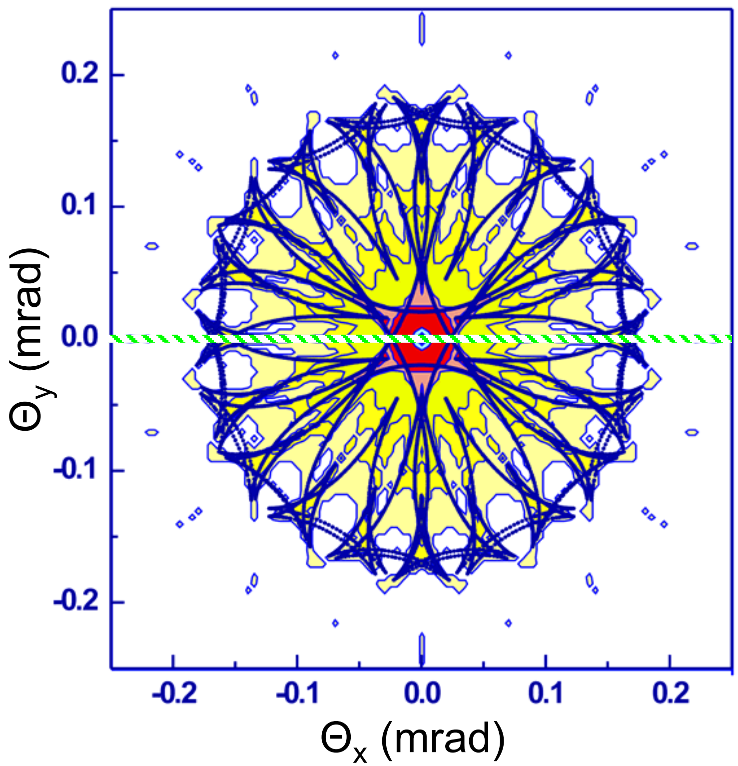


Rope length 1 µm

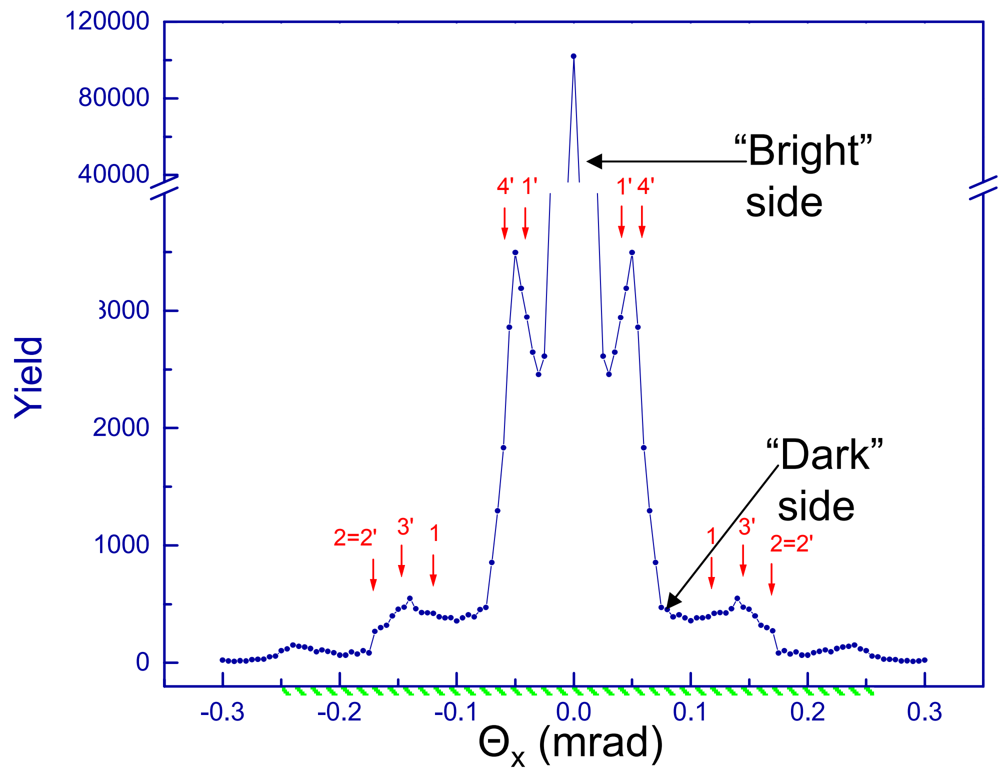
Rainbow effect after 1GeV proton channelling through a short rope of armchair SWNTs(10,10)

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

Angular distribution with rainbow lines



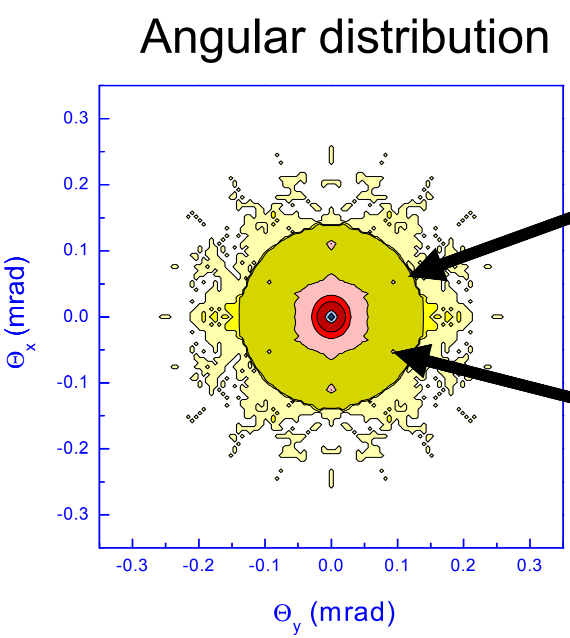
Yield of protons along Θ_x line



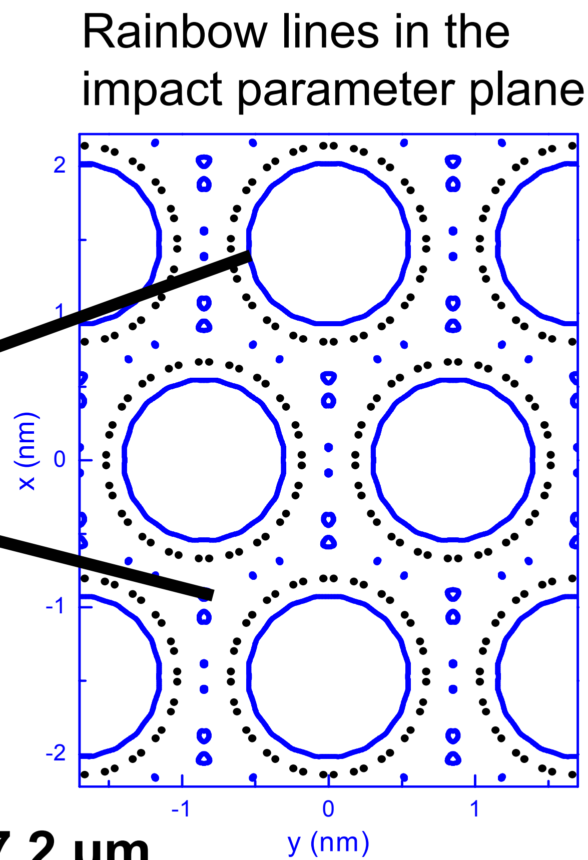
Rope length 1 μm

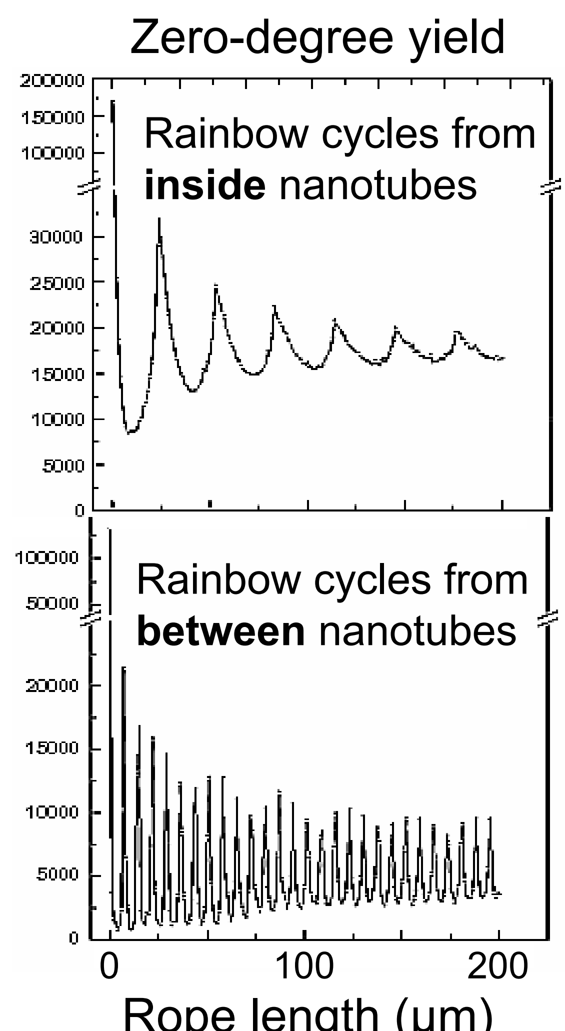
Rainbow effect after 1GeV proton channelling through <u>longer</u> ropes of <u>armchair</u> SWNTs(10,10)

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



Rope length 7.2 μm

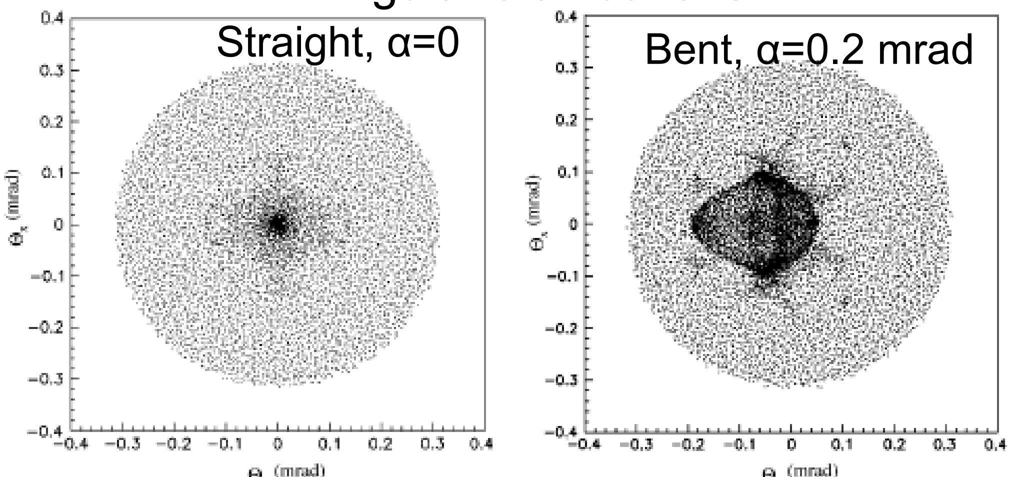




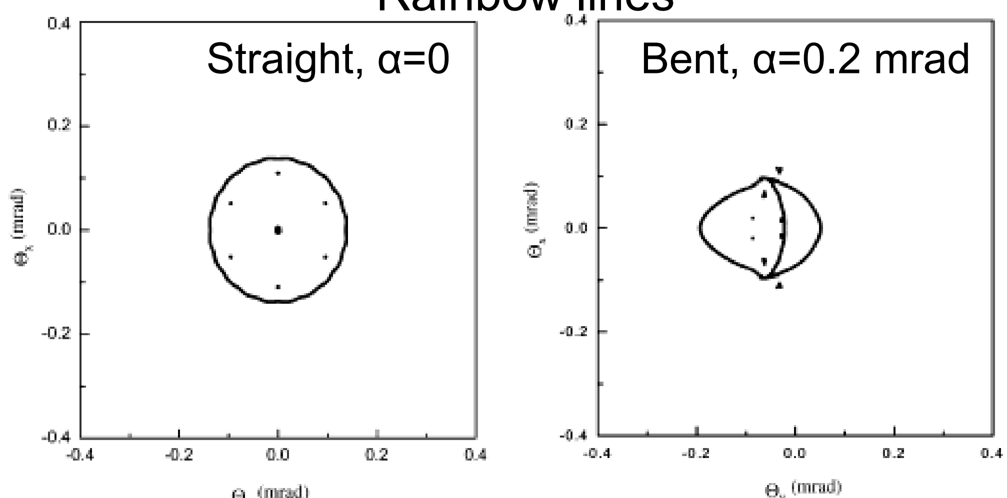
Channeling of 1 GeV protons through a bent rope of <u>armchair</u> SWNTs (10,10)

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

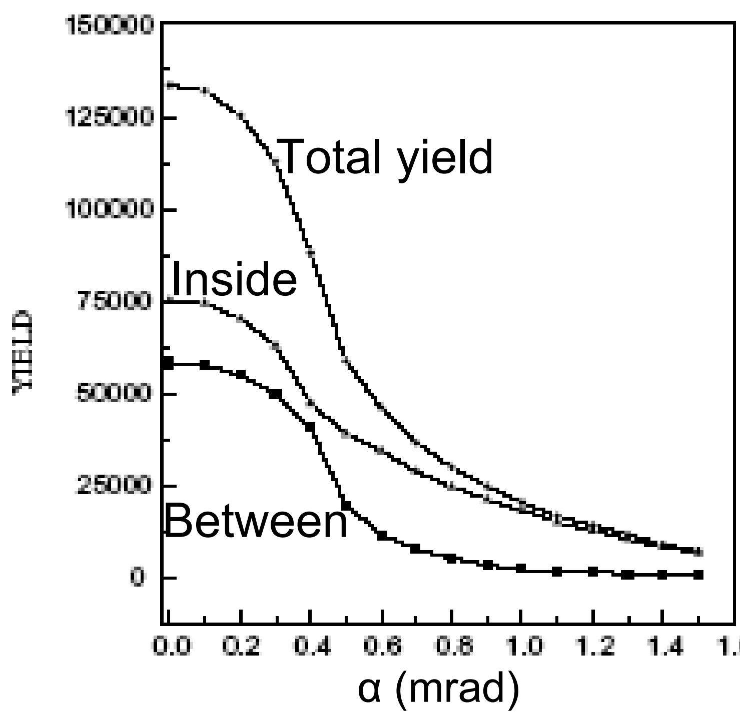
Angular distributions



Rainbow lines



Yields of protons transmitted inside and between nanotubes vs bending angle in 7 μm rope



Outline

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  - Potentials and beam deflection
  - Rainbow effect in short ropes
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  - New developments
- **Low-energy channeling** (~keV)
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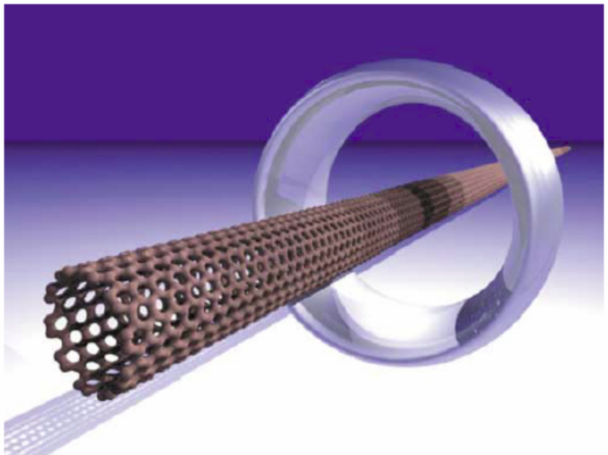
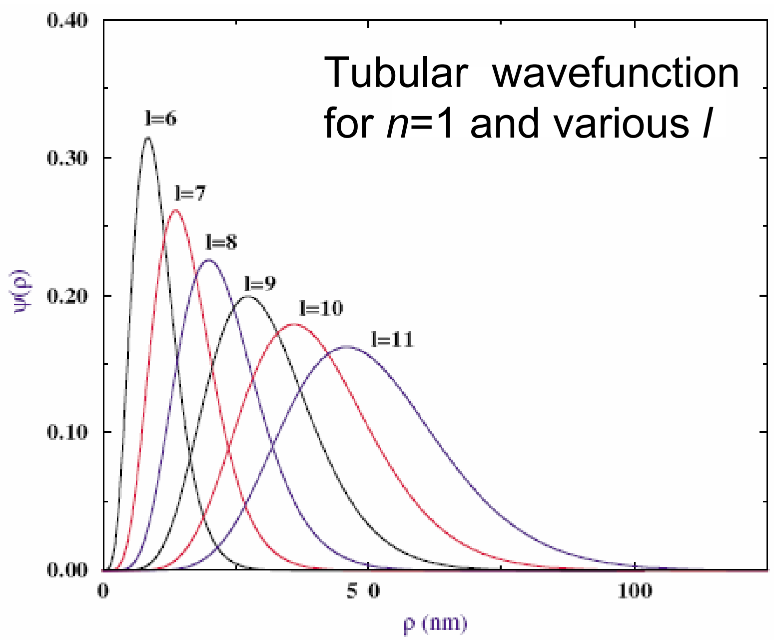
  - Related problems
- **Outlook**

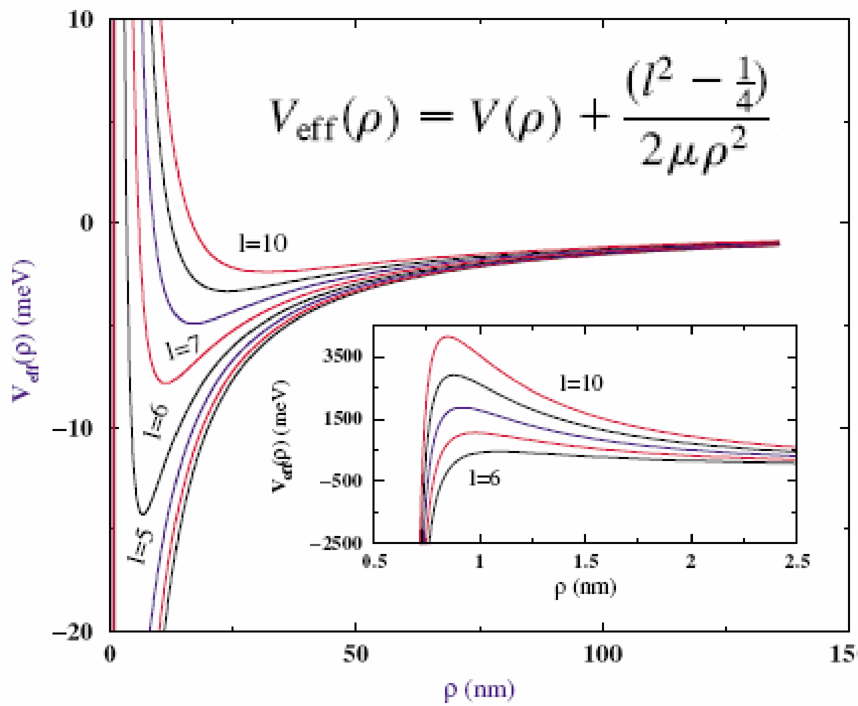
Electron image states around carbon nanotubes

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





Effective potential around SWNT (10,10)



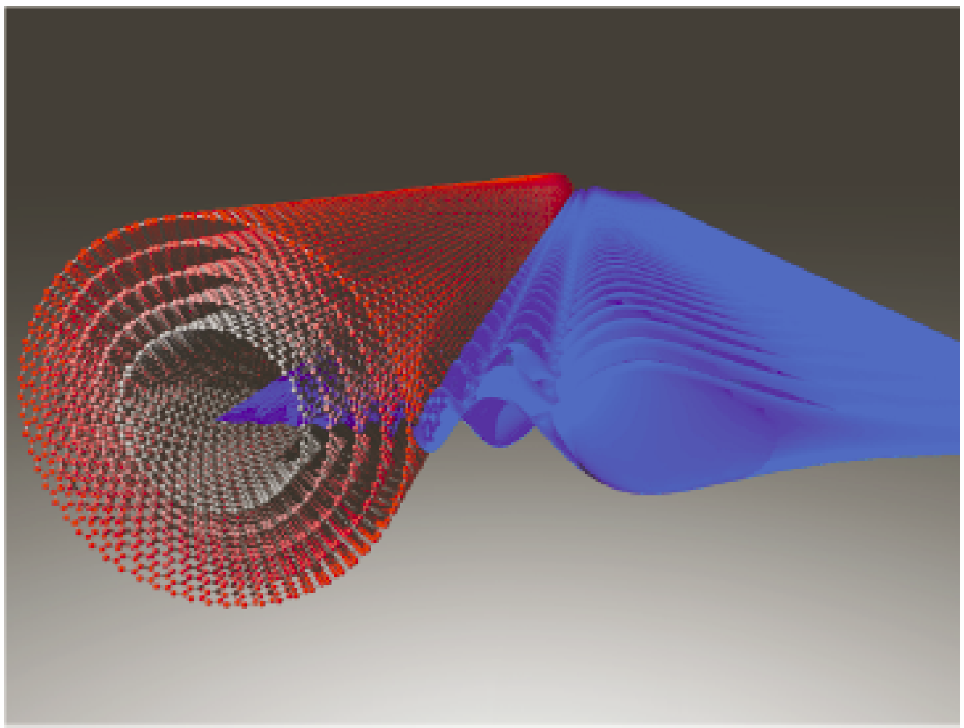
Approximate image potential

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

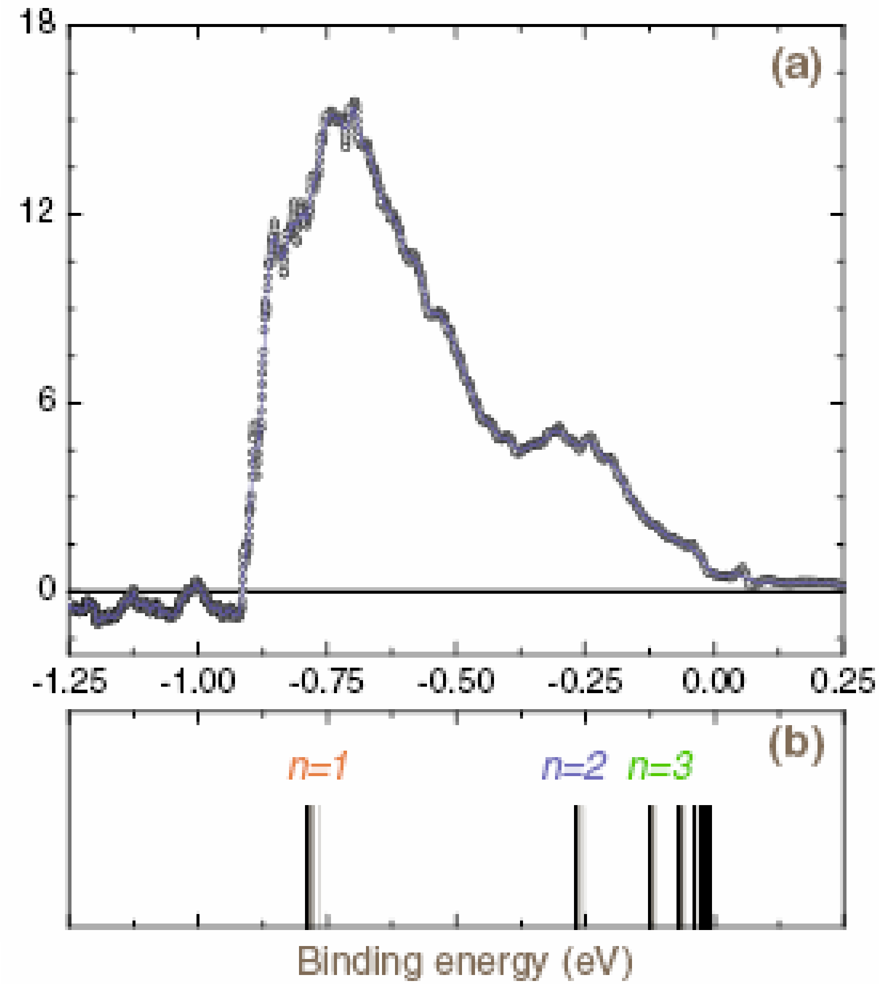
Electron image states around carbon nanotubes

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

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

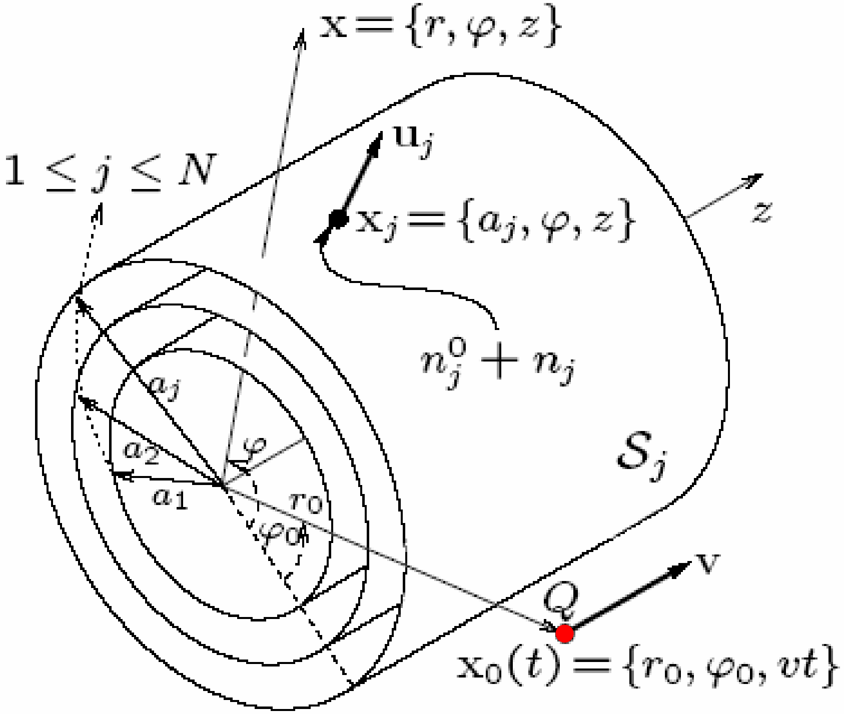


Photoelectron signal from image state



2D hydrodynamic model of electron response

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



$$\frac{\partial n_j(\mathrm{x}_j,t)}{\partial t} = -n_j^0 \nabla_j \cdot \mathrm{u}_j(\mathrm{x}_j,t)$$

$$\frac{\partial \mathrm{u}_j(\mathrm{x}_j,t)}{\partial t} = \nabla_j \Phi(\mathrm{x},t)|_{r=a_j} - \frac{\alpha_j}{n_j^0}\nabla_j\, n_j(\mathrm{x}_j,t) + \frac{\beta}{n_j^0}\nabla_j\left[\nabla_j^2\, n_j(\mathrm{x}_j,t)\right] - \gamma_j \mathrm{u}_j(\mathrm{x}_j,t)$$

$$\Phi(\mathrm{x},t) = \frac{Q}{\|\mathrm{x}-\mathrm{x}_0(t)\|} - \sum_j \int_{\mathcal{S}_j} d^2\mathrm{x}'_j\, \frac{n_j(\mathrm{x}'_j,t)}{\|\mathrm{x}-\mathrm{x}'_j\|}$$

Stopping power

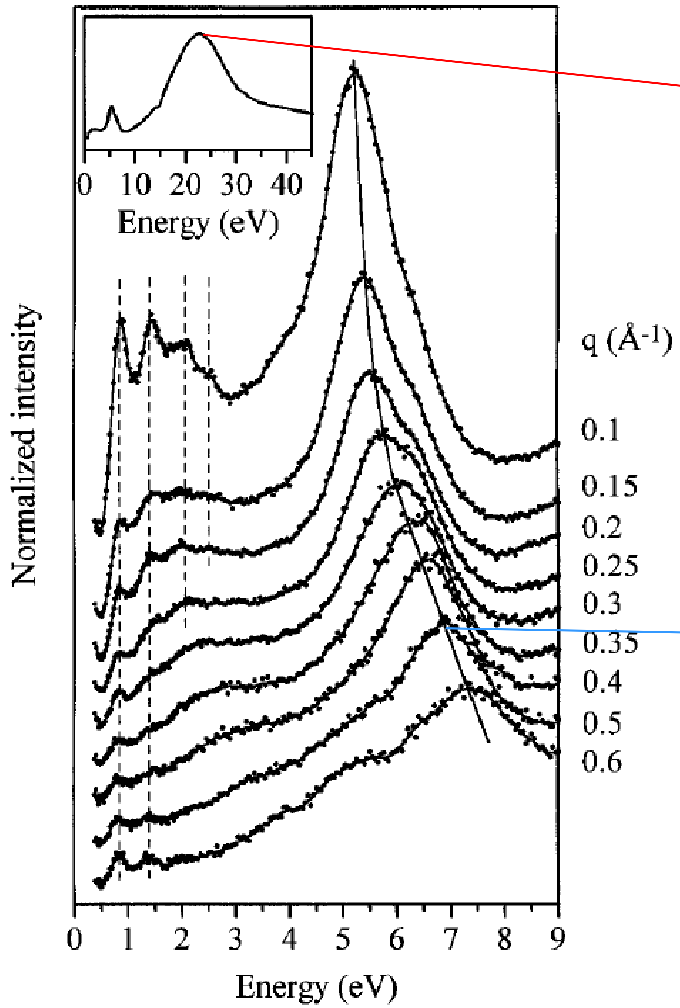
$$S = Q\frac{\partial \Phi_{ind}}{\partial z}\Big|_{\mathrm{x}=\mathrm{x}_0(t)}$$

Self-energy (image potential)

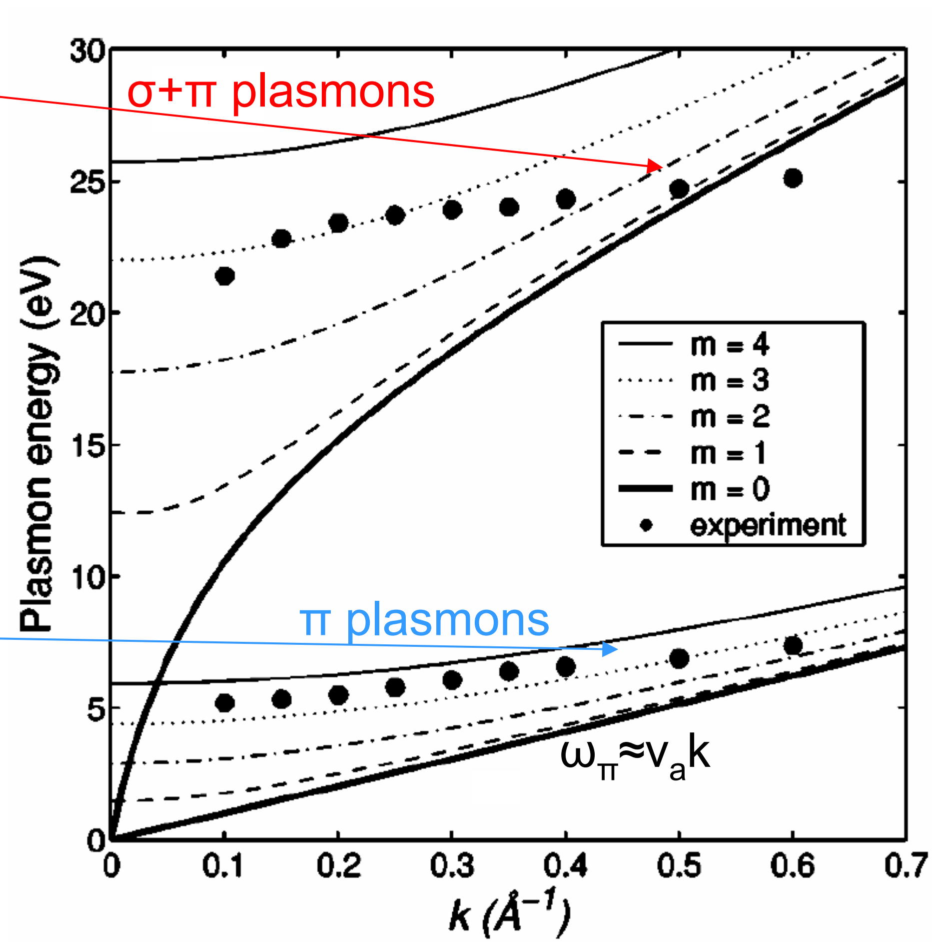
$$E_s = -\frac{Q}{2}\Phi_{ind}\Big|_{\mathrm{x}=\mathrm{x}_0(t)}$$

Plasmon spectra: σ and π electrons on SWNT

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

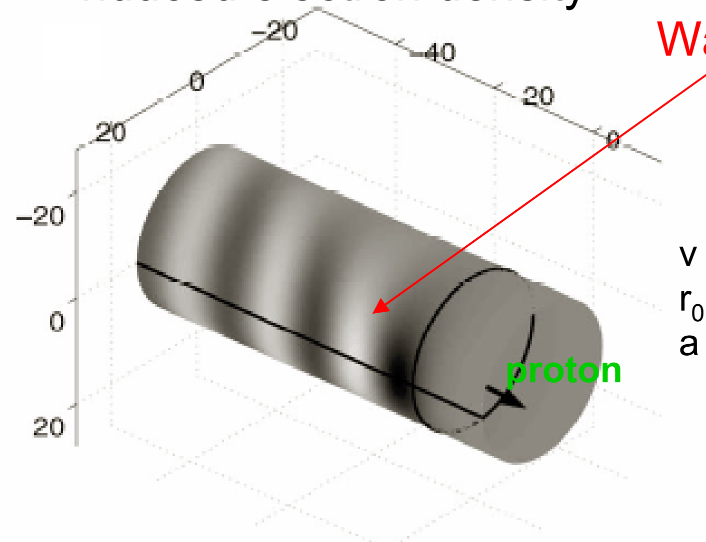


Theoretical plasmon dispersion:
Two-fluid model



Dynamic polarization of electrons on SWNT by proton

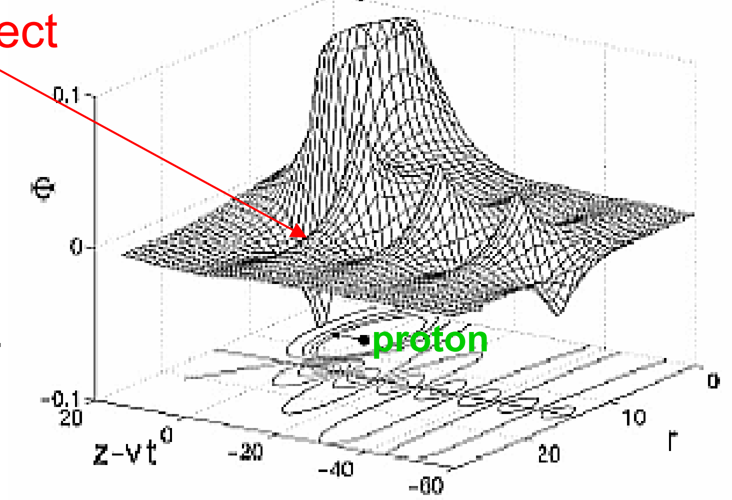
Induced electron density



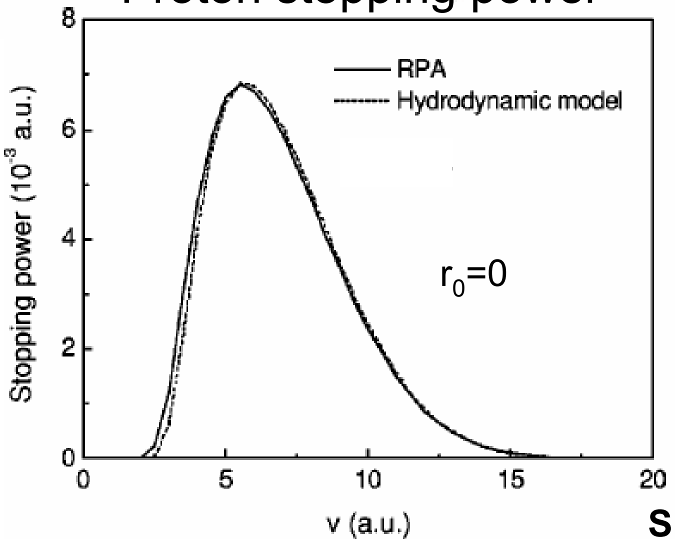
Wake effect

v = 3 a.u.
$r_0 = a/2$
a = 13 a.u.

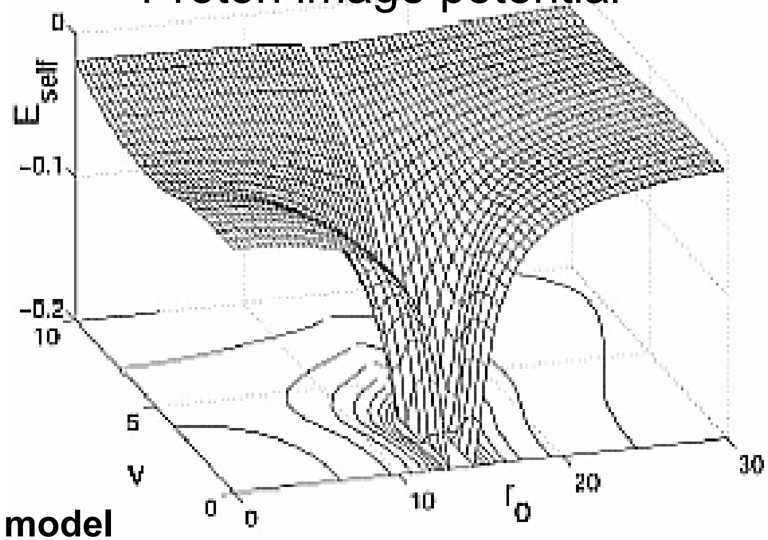
Total potential



Proton stopping power



Proton image potential

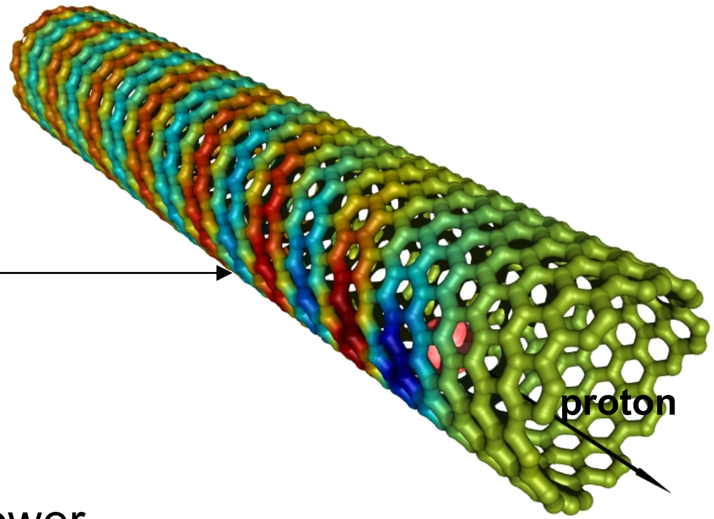


Single-fluid model

Dynamic polarization of electrons on SWNT by proton

Single-fluid model

Wake in induced electron density



v = 3 a.u., r_0 = a/2

Stopping power

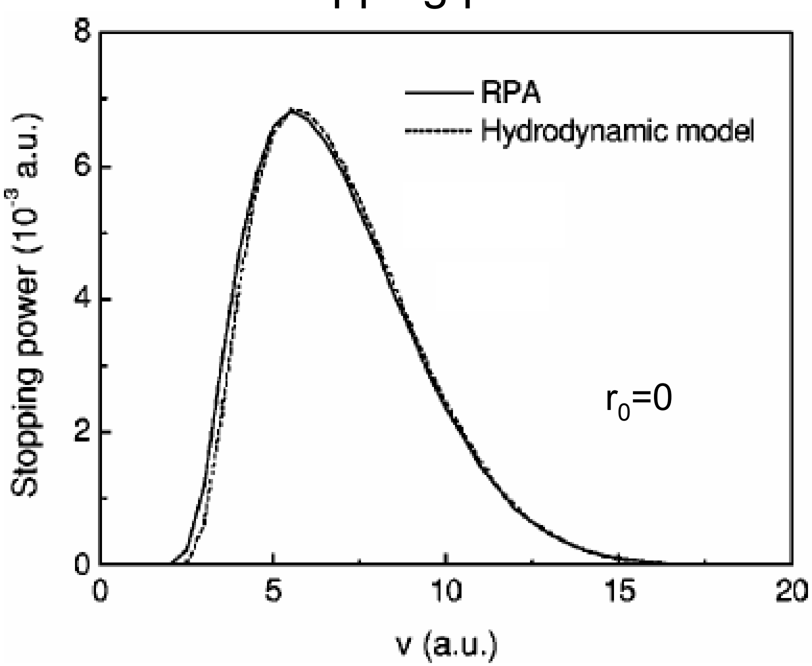
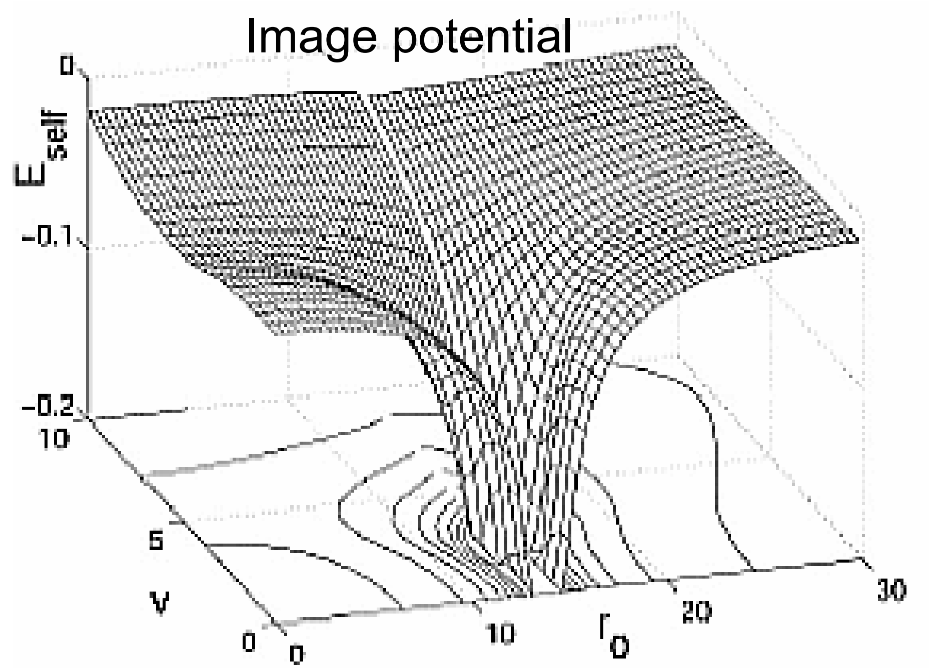
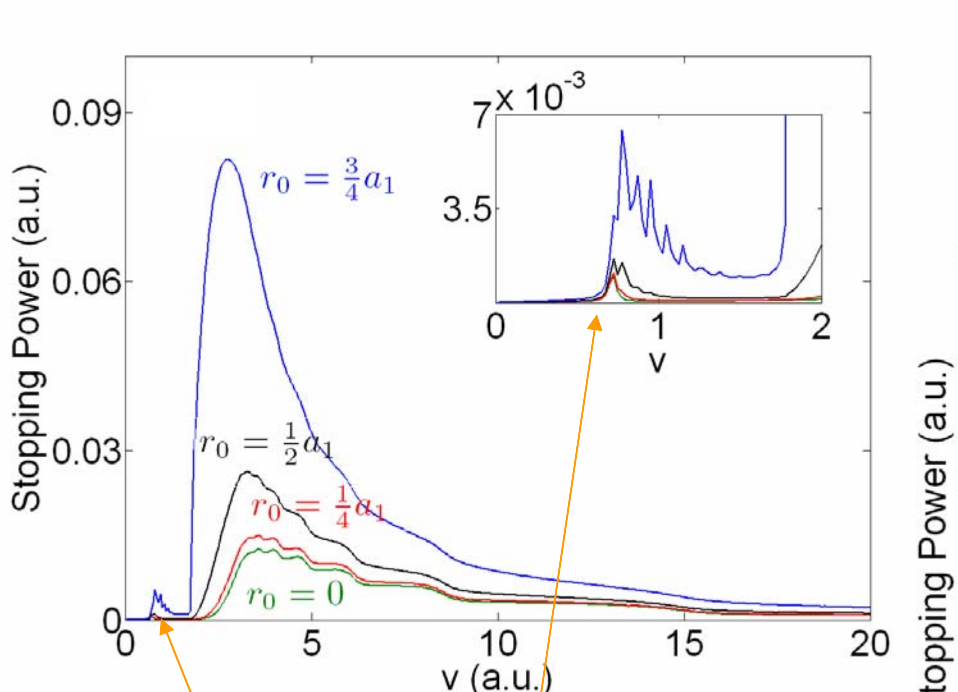


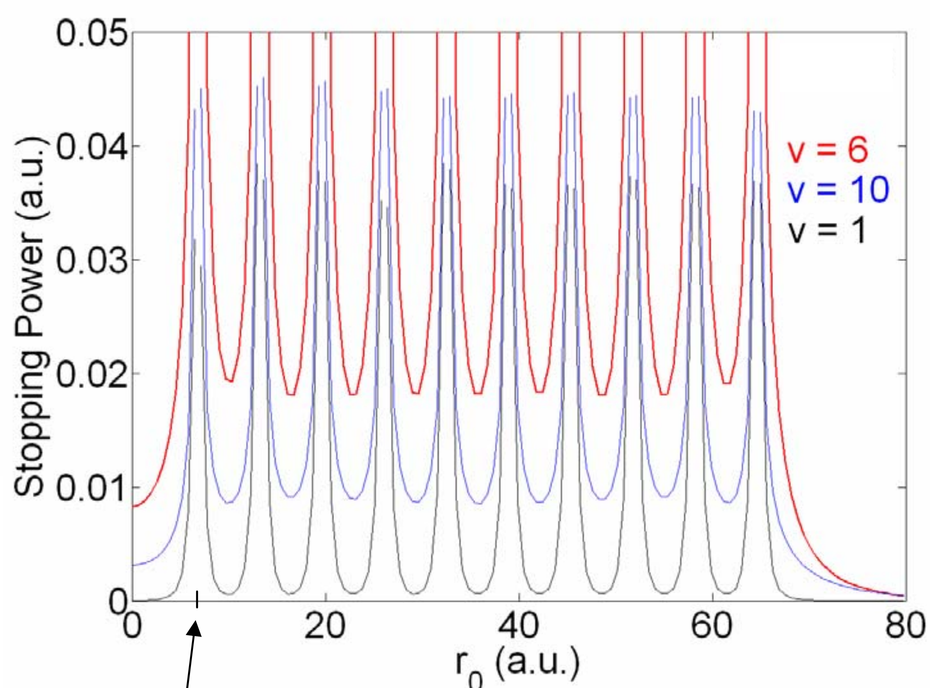
Image potential



Proton stopping power for MWNT with N = 10 walls



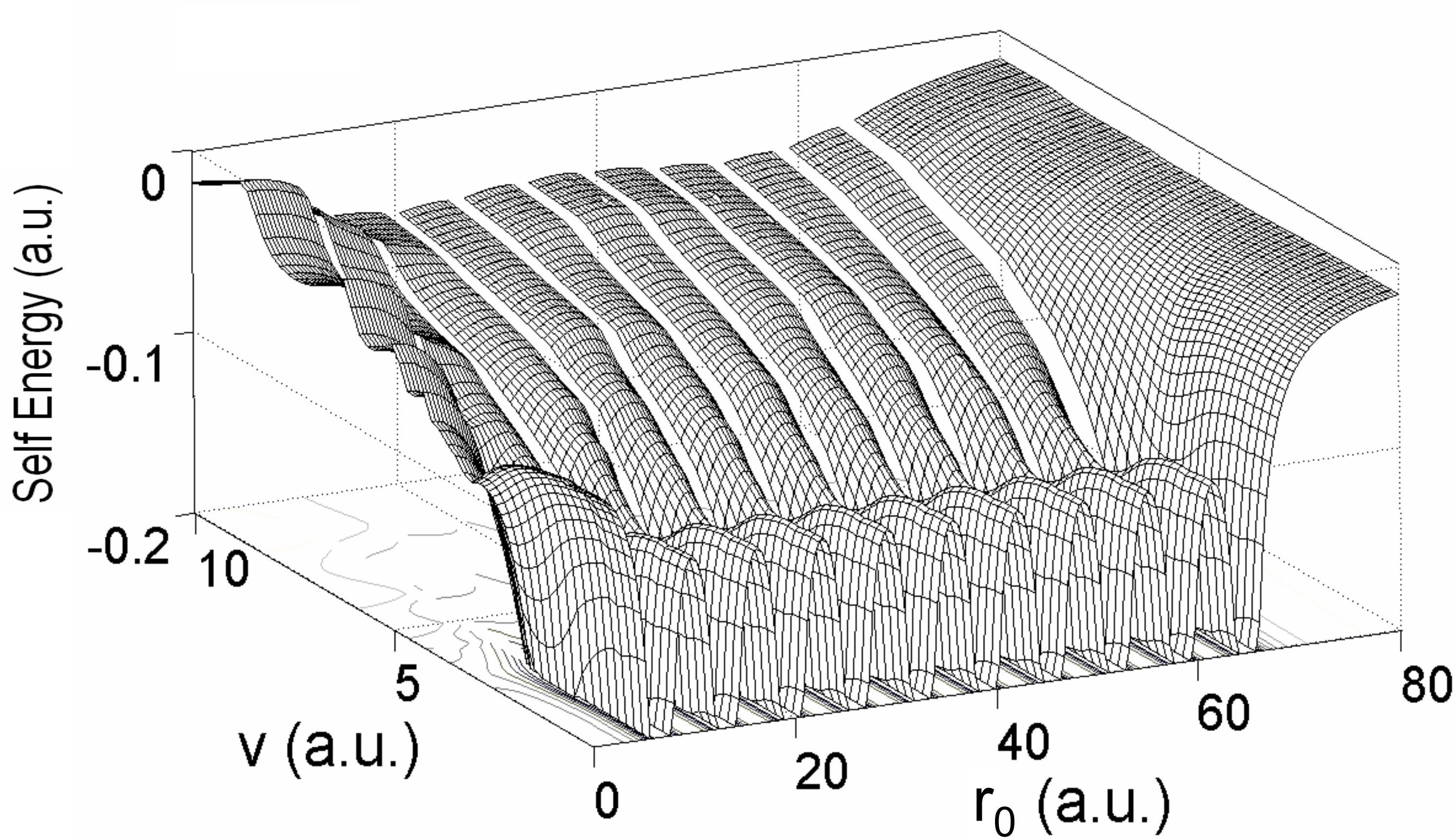
Stopping power vs radial position r_0



$a_1 \approx 6.8$ a.u.

Calculations done with **two-fluid model**: Notice low-speed features due to quasi-acoustic π plasmons having dispersion relation $\omega_\pi \approx v_a k$ with the acoustic speed $v_a = (3\pi n_0/8)^{1/2} \approx 0.7$ a.u..

Proton self energy (image potential) for MWNT with *N* = 10 walls (single-fluid model)



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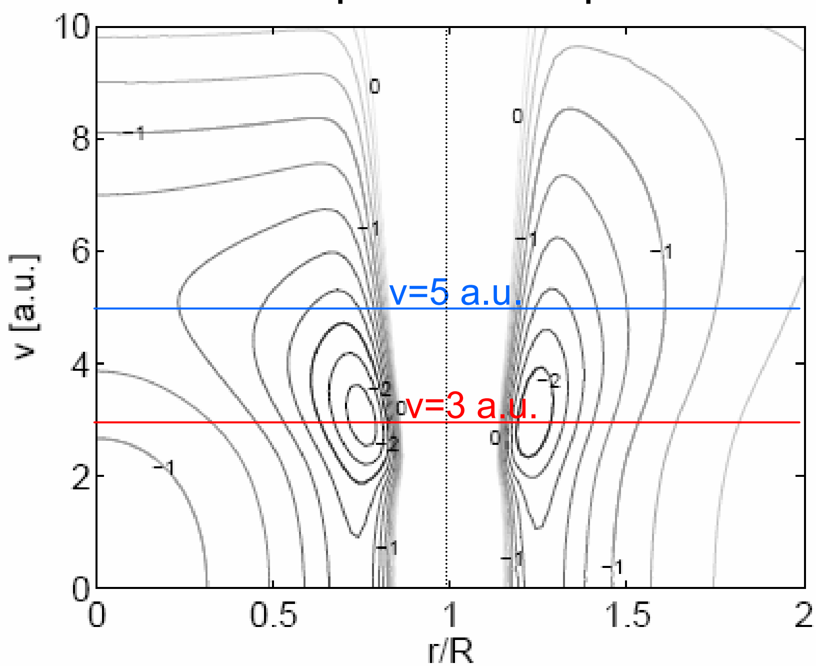
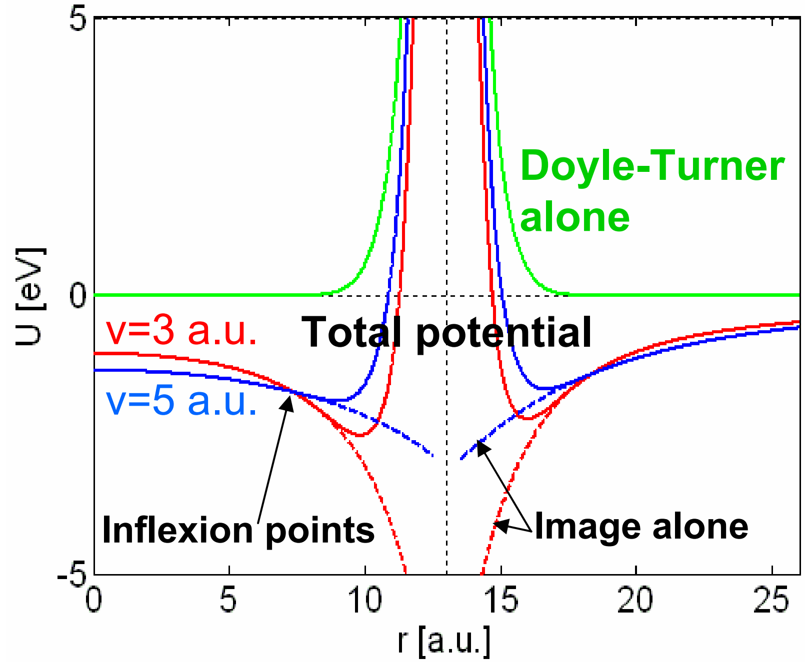
Total potential for proton moving parallel to a chiral SWNT(11,9) with image and Doyle-Turner potentials

Nanotube radius ≈ 13 a.u.

Contour plot of total potential





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

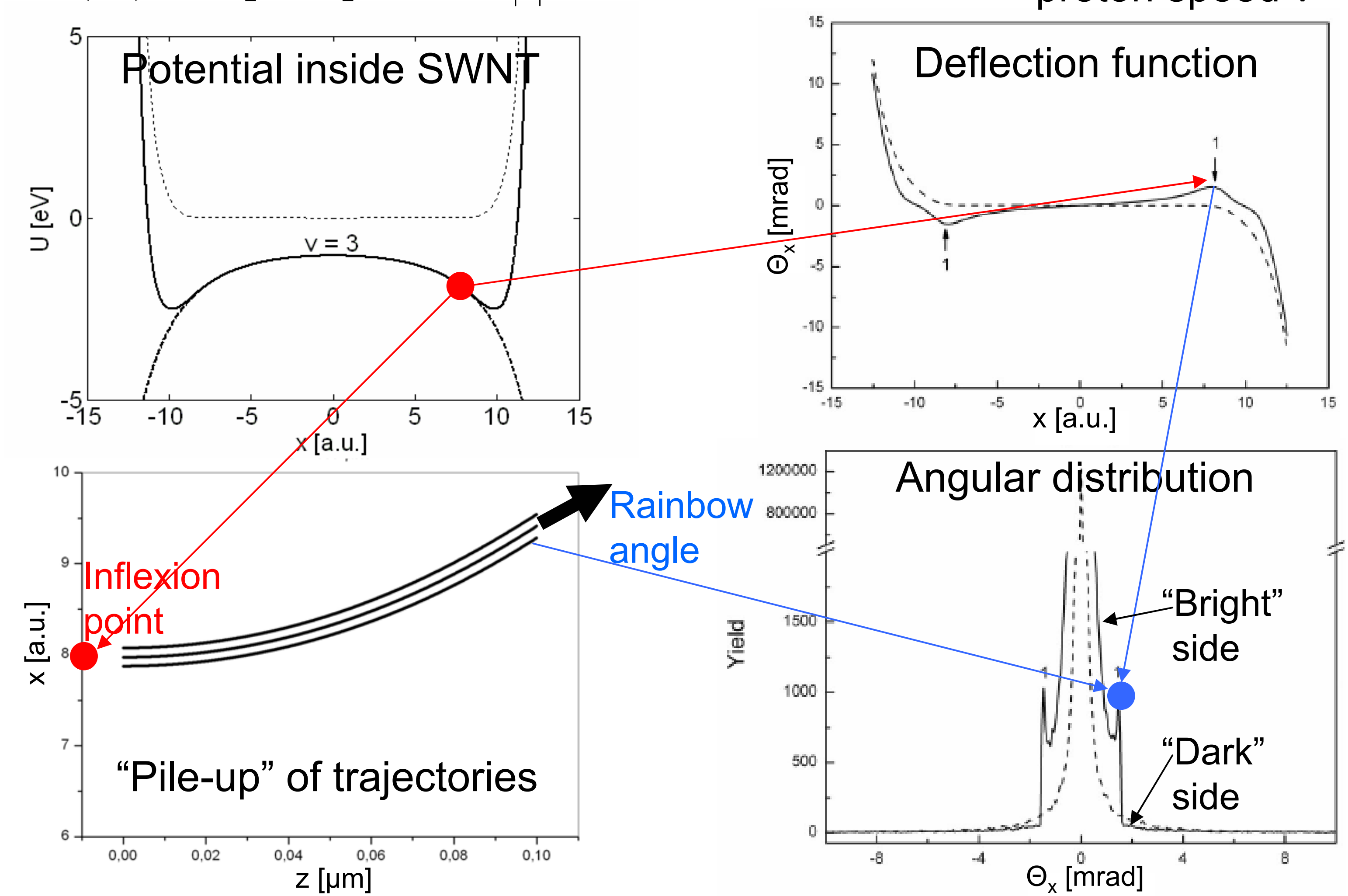
$$\omega_m^2(k) = (k^2 + m^2/R^2)\left[v_s^2 + 4\pi n_0 R\, I_m(kR) K_m(kR)\right], \quad r_< = \min(r, R),\ r_> = \max(r, R)$$

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

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

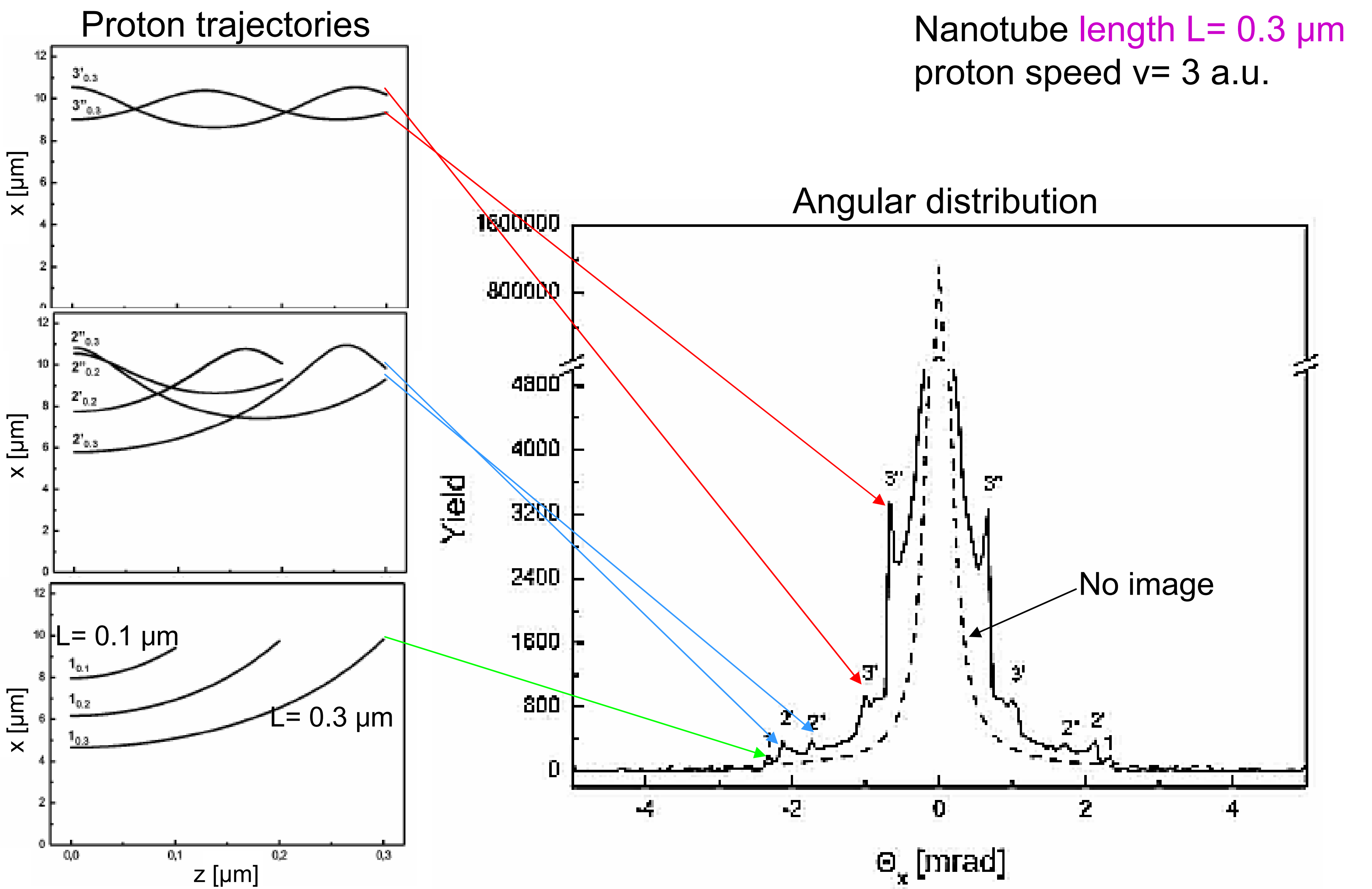
$$J = \left(\frac{L}{2E}\right)^2 \frac{1}{2r}\frac{d}{dr}\left[\frac{dU(r)}{dr}\right]^2 = 0 \Rightarrow \sigma = \frac{1}{|J|} \to \infty$$

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



Formation of multiple rainbows in chiral SWNT(11,9)

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



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

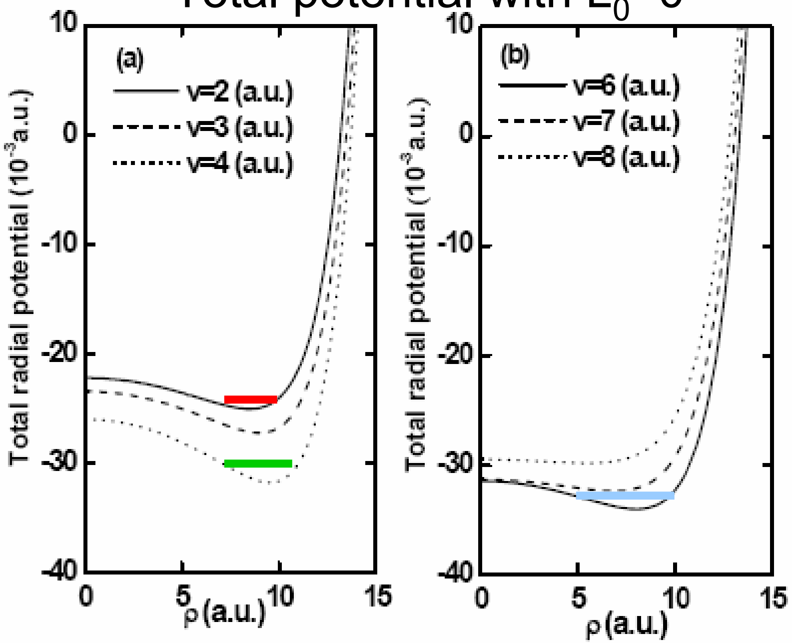
D.P. Zhou *et al.*, *Phys. Rev.* A 72 (2005) 23202

Nanotube radius =20 a.u.

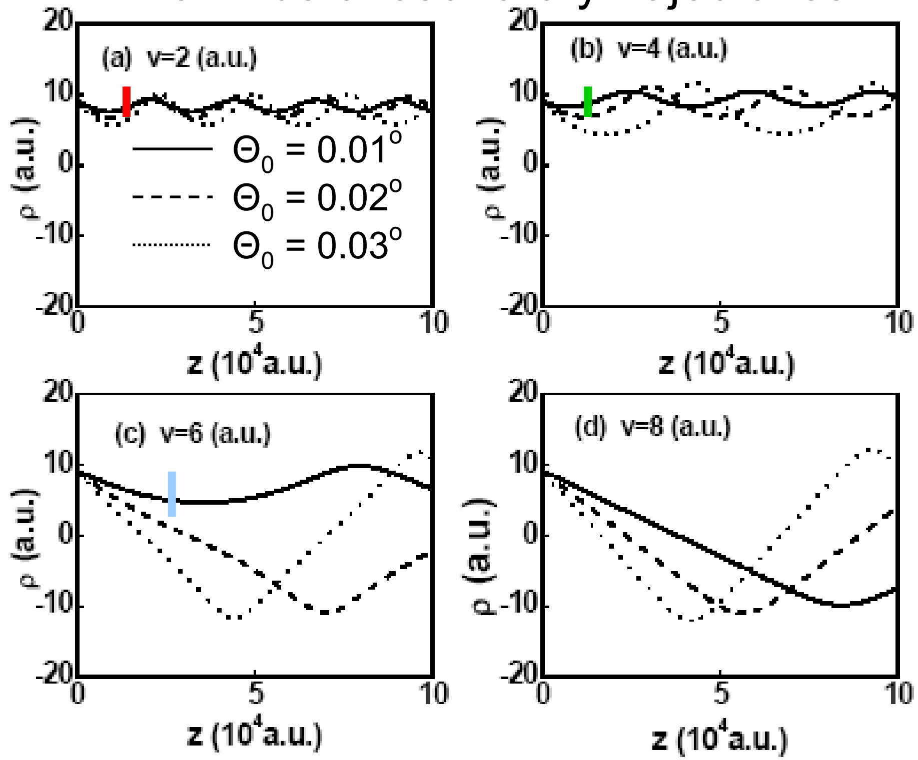
$$M\ddot{\rho} = F_{\rho}^{(n)} + F_{\rho}^{(p)} + \frac{L_0^2}{M\rho^3}, \qquad M\ddot{z} = F_z^{(p)}, \qquad M\rho^2\dot{\phi} = L_0,$$

Moliere & image forces, stopping force; angular momentum

Total potential with L_0=0



Two kinds of oscillatory trajectories

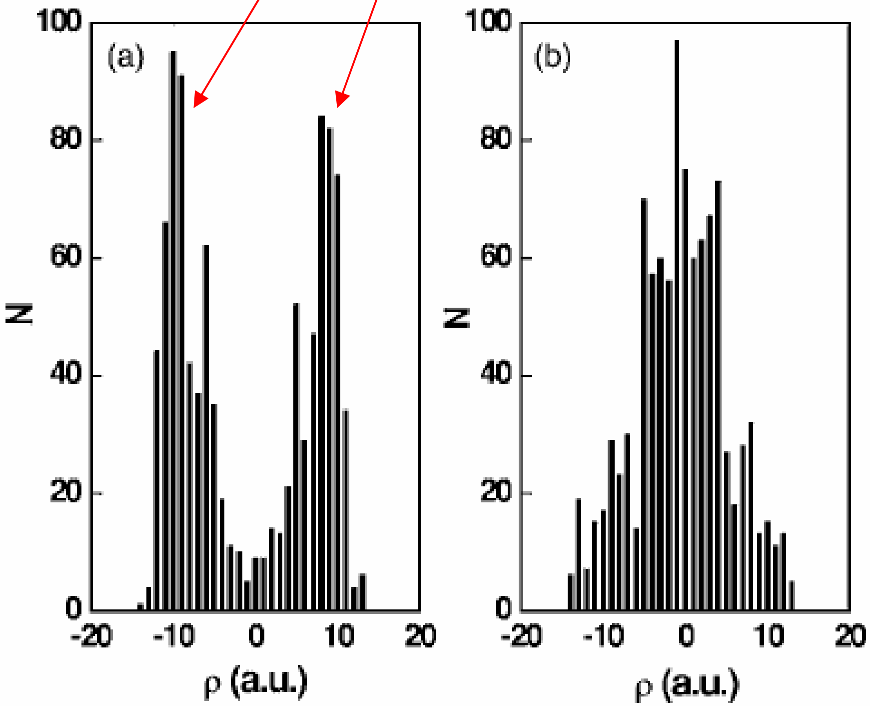


Creation of hollow nano-beam of protons after channelling through a SWNT due to image force

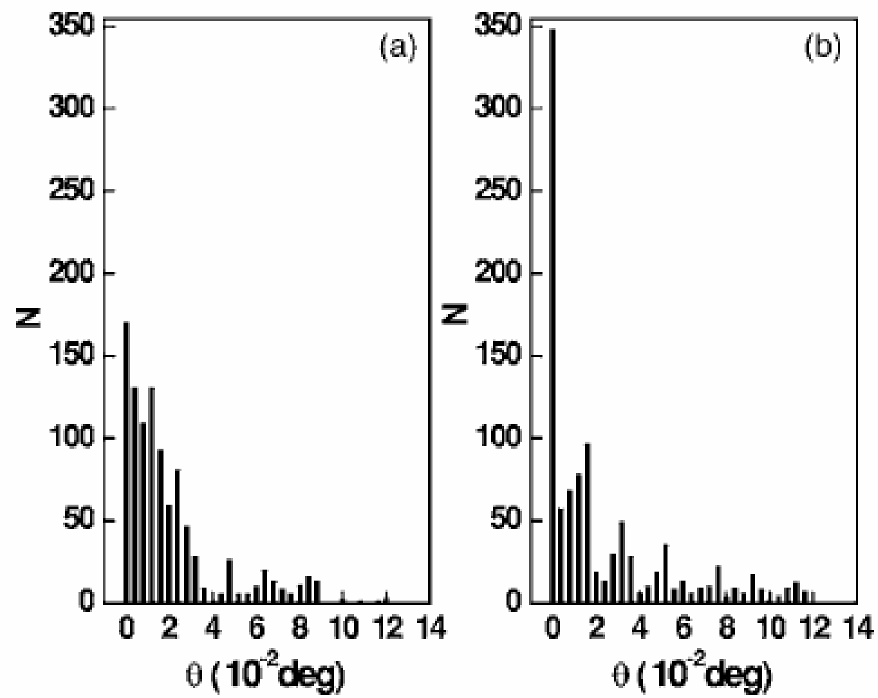
D.P. Zhou *et al.*, *Phys. Rev.* A 72 (2005) 23202

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_2^+ channelling in SWNT

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

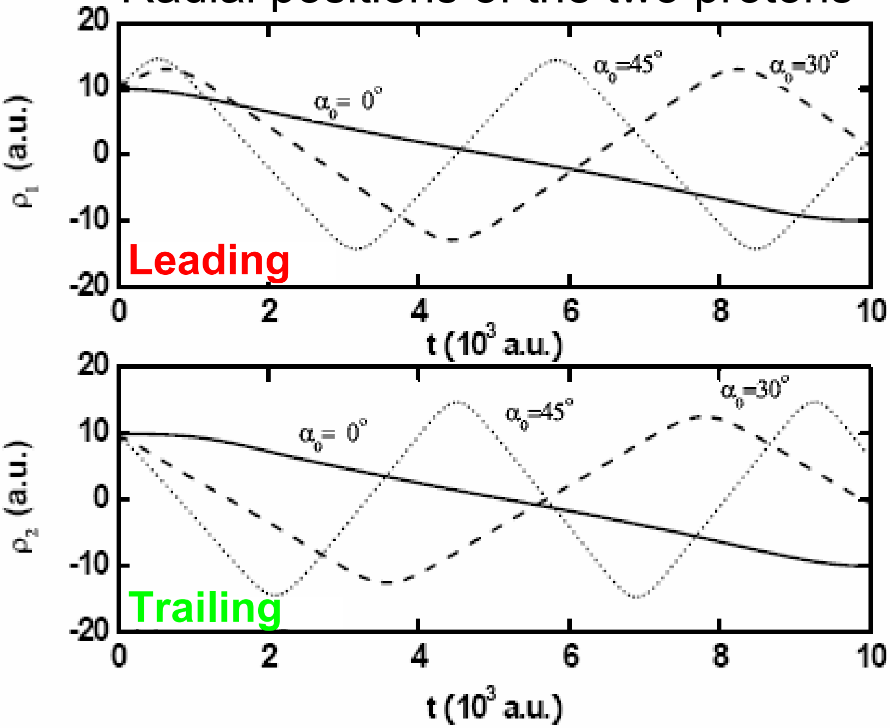
Solve classical equations of motion:

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

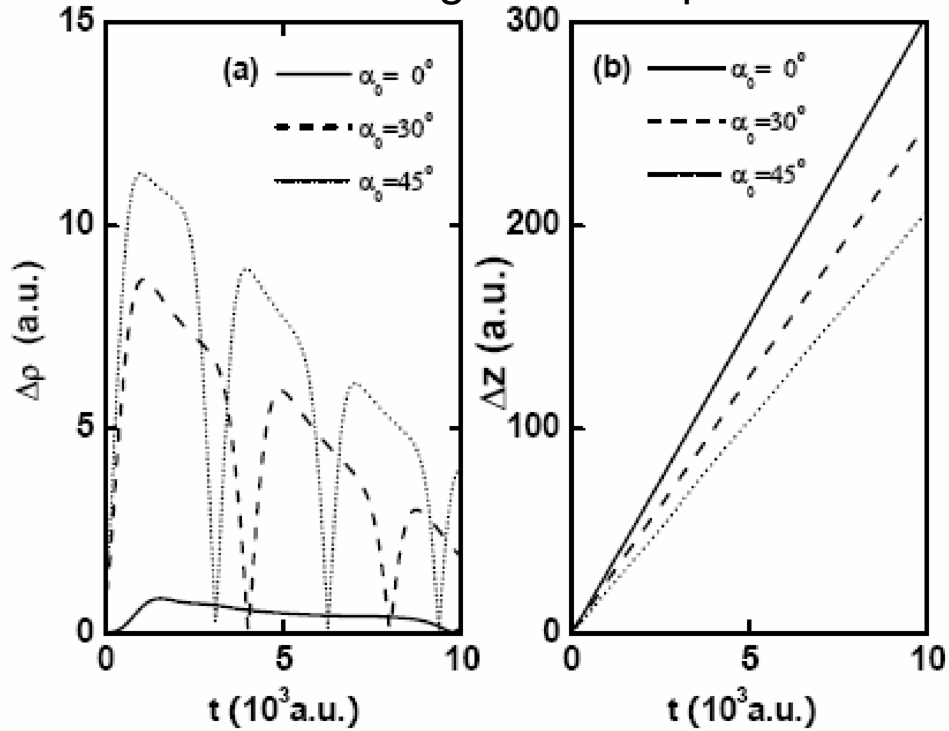
Forces: Coulomb, polarization, Moliere

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

Radial positions of the two protons



Radial and longitudinal separations



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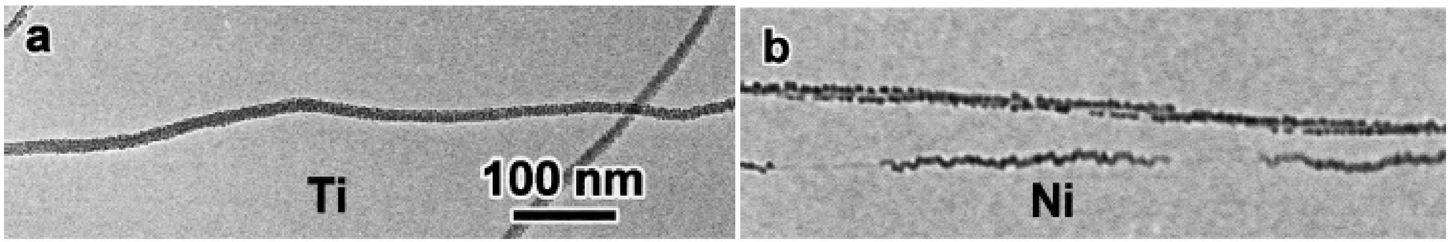
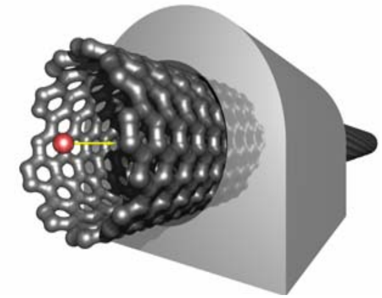
Dynamic polarization of SWNT coated by metal

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





Stopping power in SWNT with a=7Å

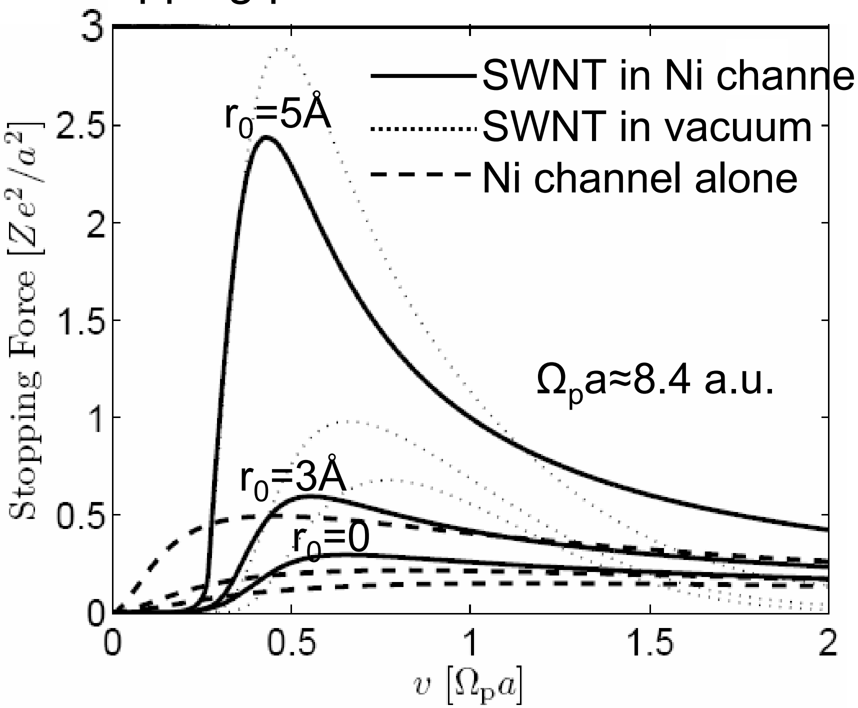
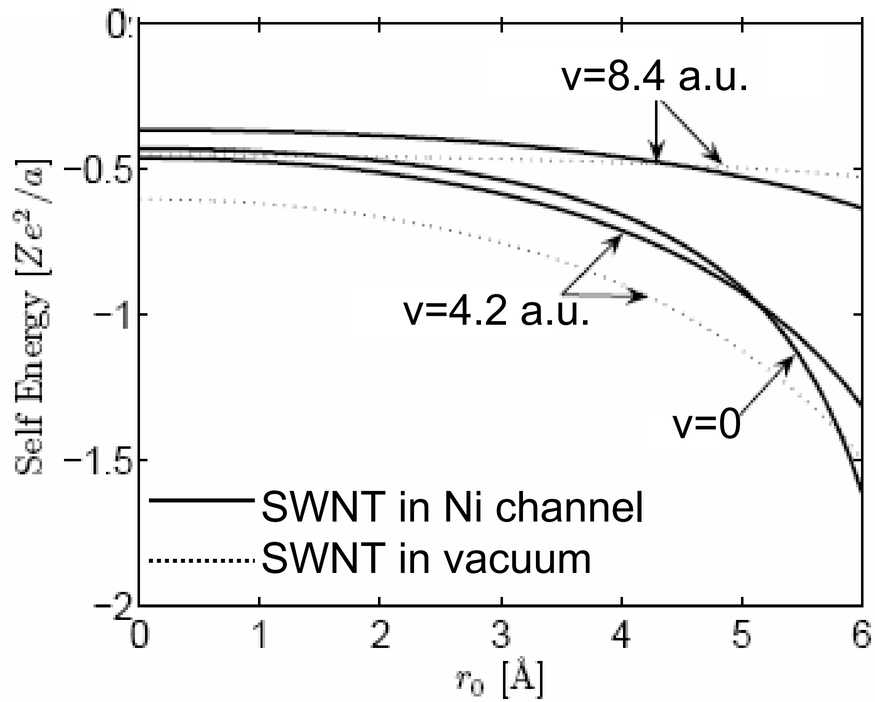
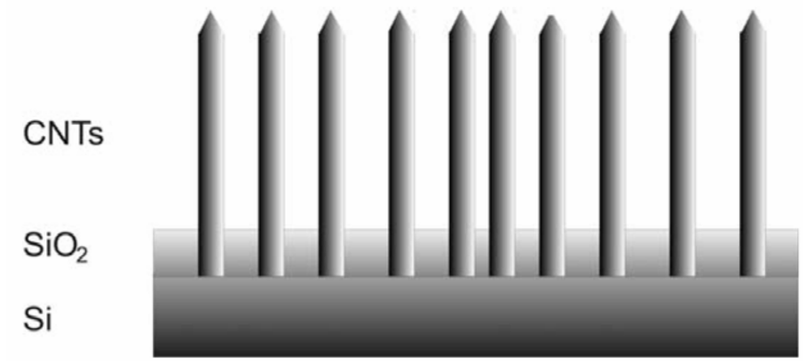


Image potential in SWNT with a=7Å



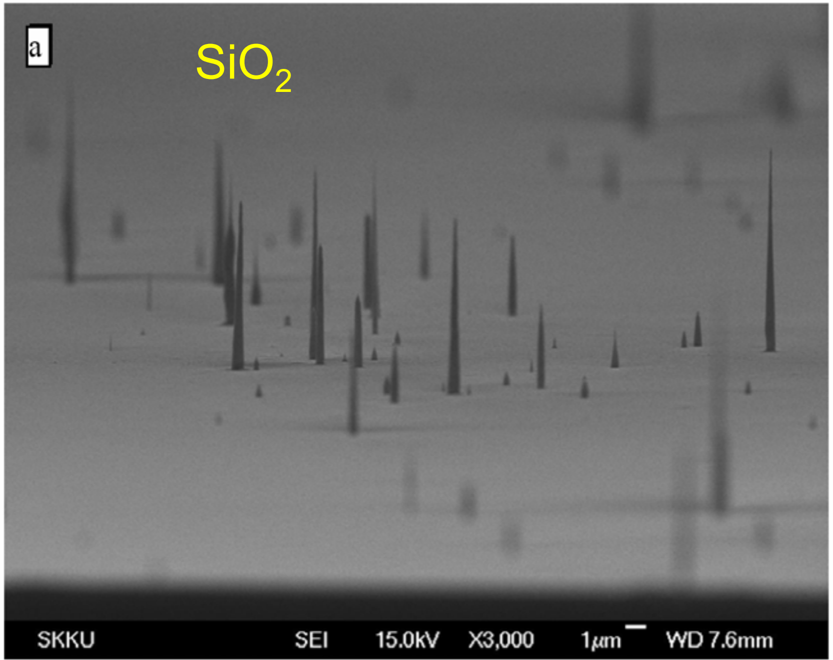
Growth of CNTs in etched ion tracks in SiO_2

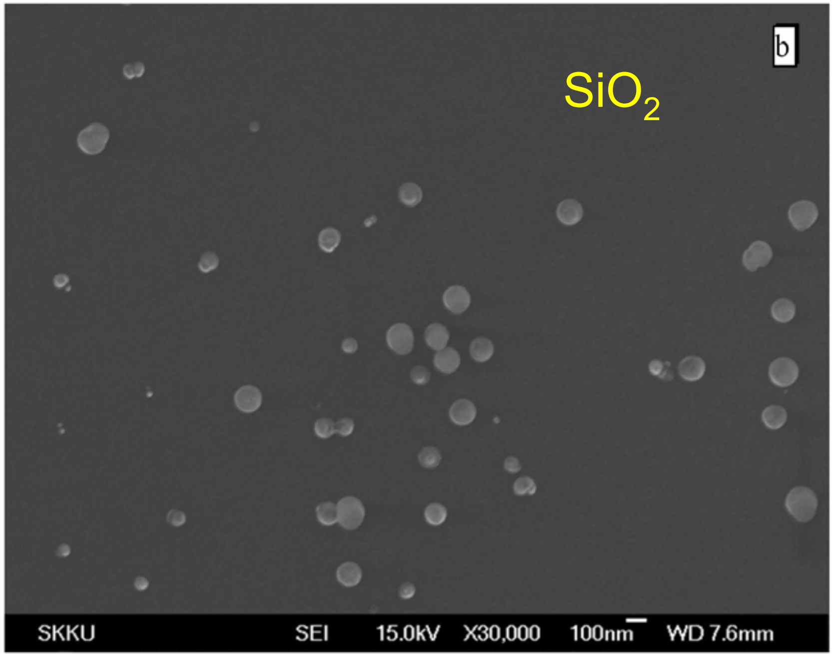
A.S. Berdinsky *et al., in press* (2006)



Side view showing pointed tips

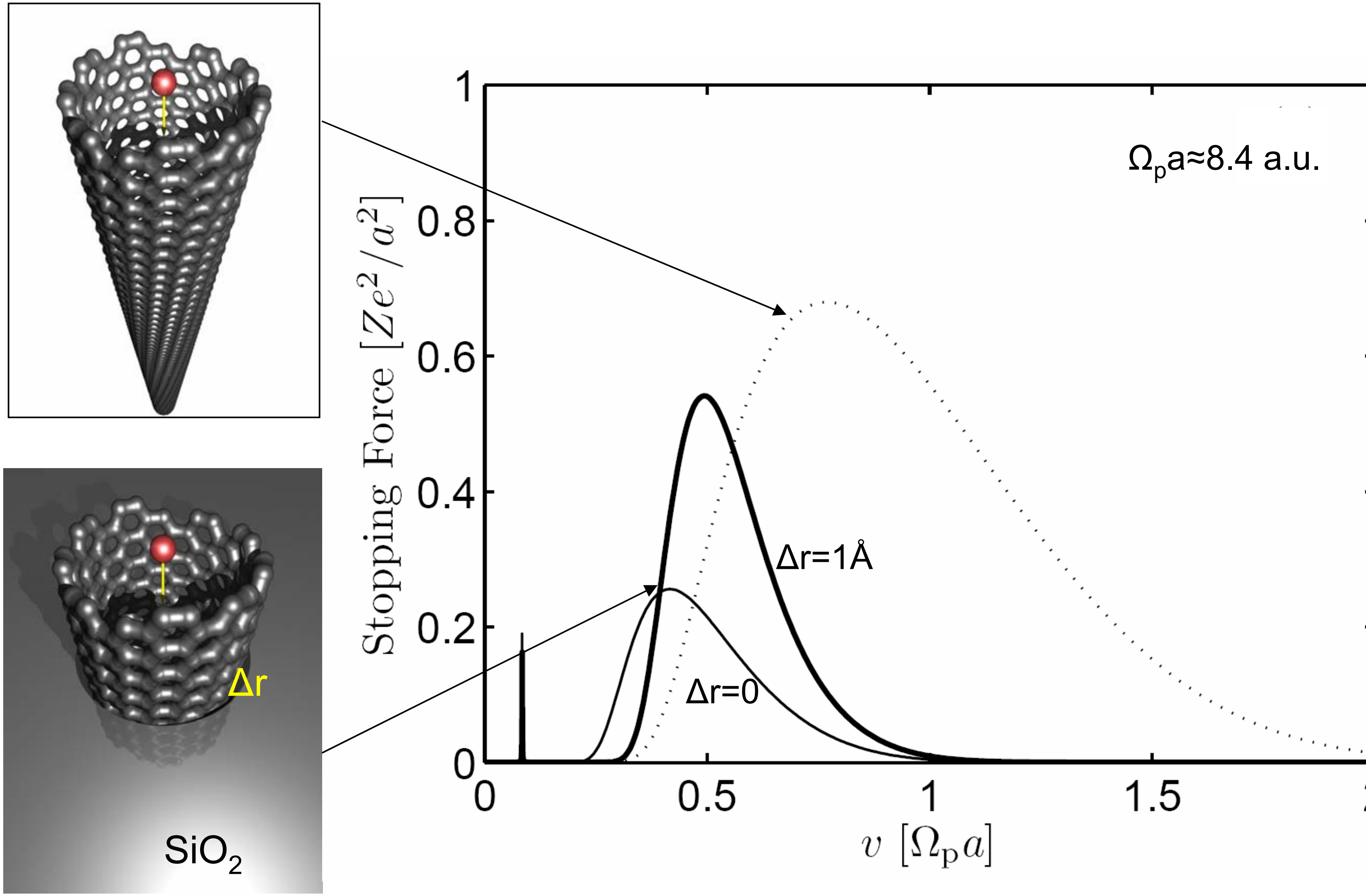
Top view showing alignment





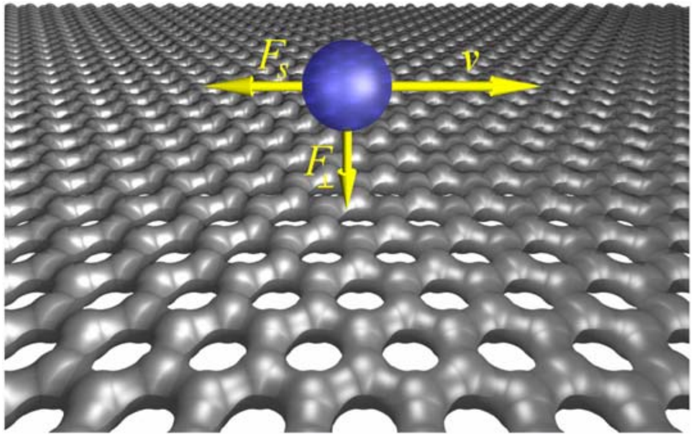
Proton stopping power in SWNT in SiO_2 channel

D.J. Mowbray *et al., Phys. Rev.* B 74 (2006) 15 November



Planar channeling in Highly Oriented Pyrolytic Graphite

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

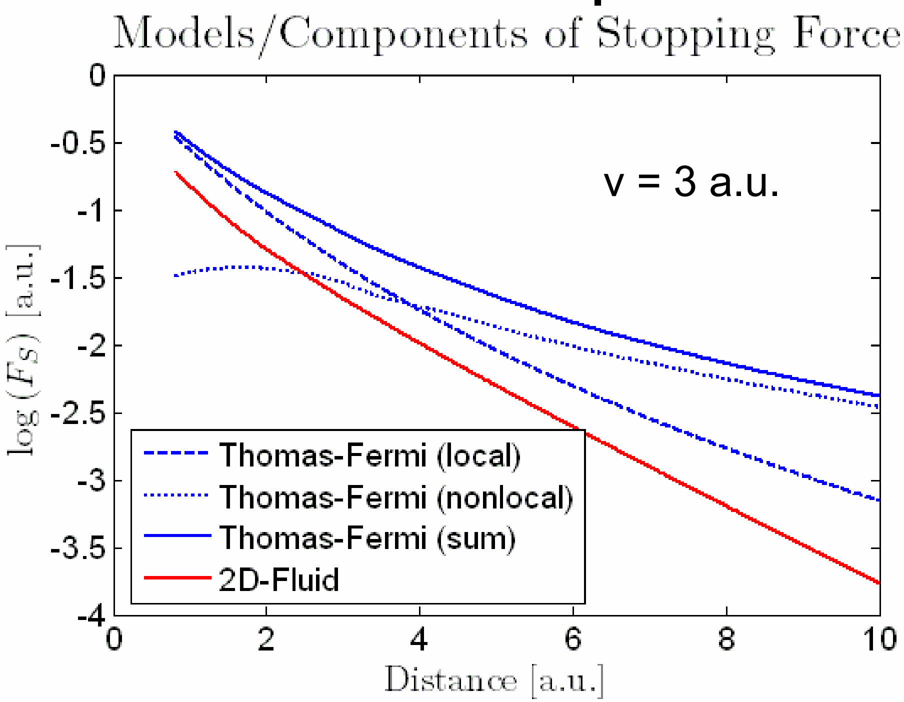


For **single** graphene sheet, calculate stopping power and image force using Kitagawa's dielectric function:

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

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

Compare 3D and 2D electron-gas models



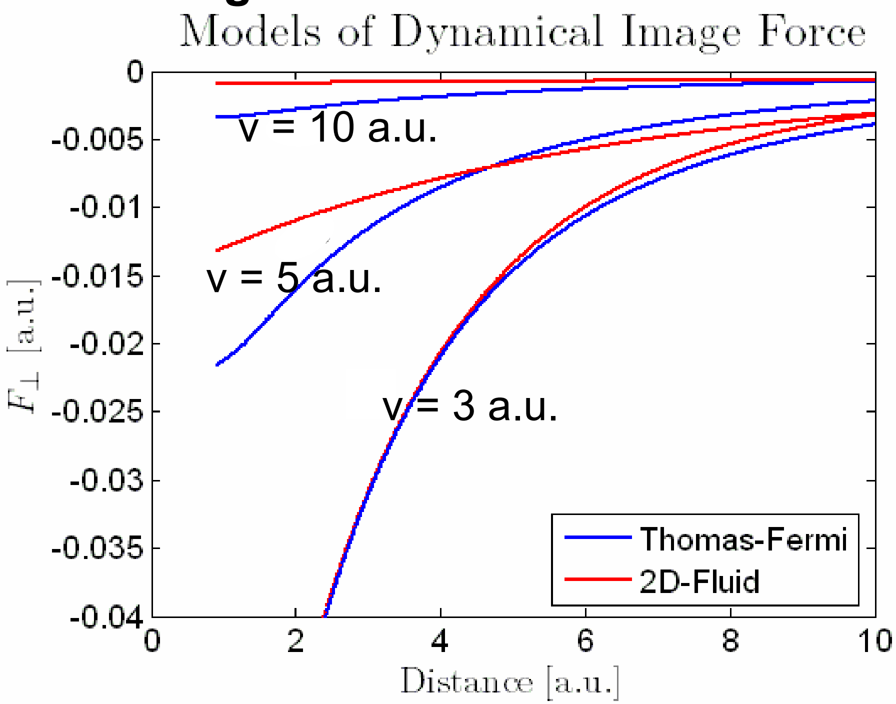
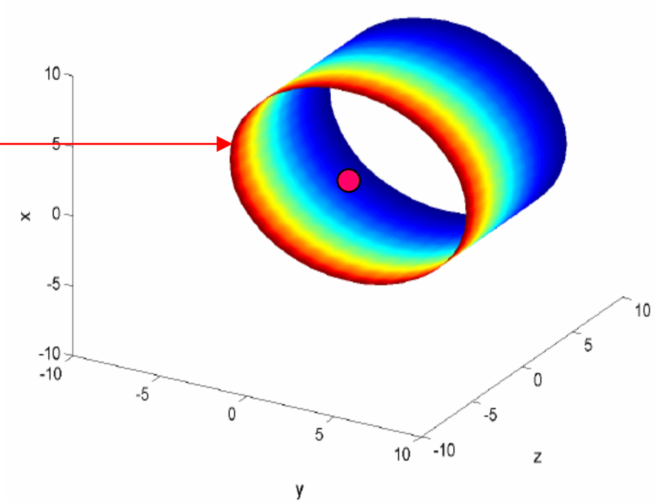


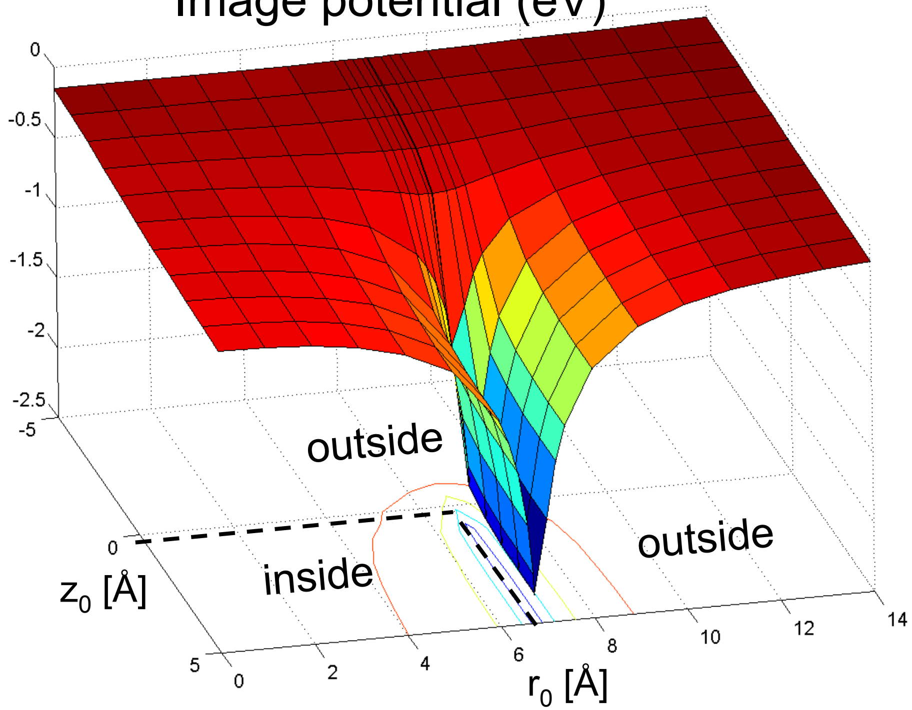
Image potential of slow ion near open end of a SWNT

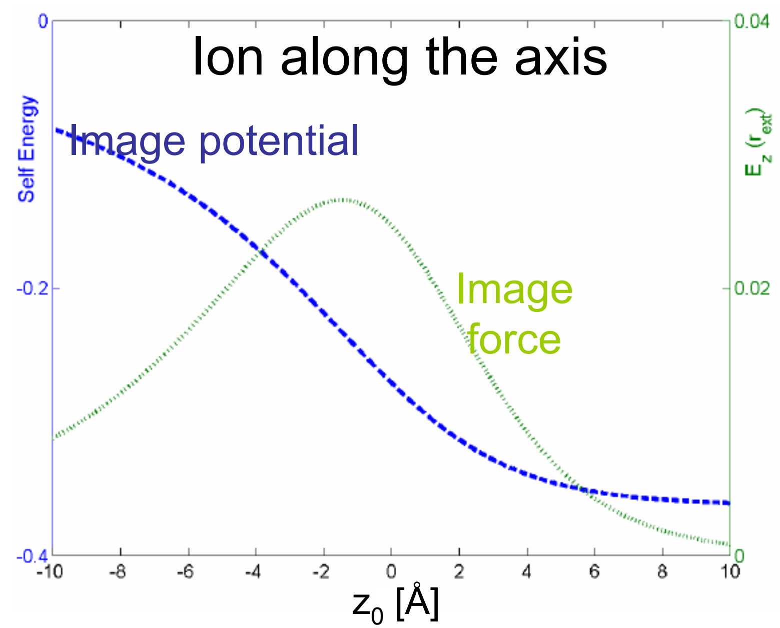
K. Whyte and Z.L. Miskovic, in preparation

Solve integral equation for induced electron density ***n***

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







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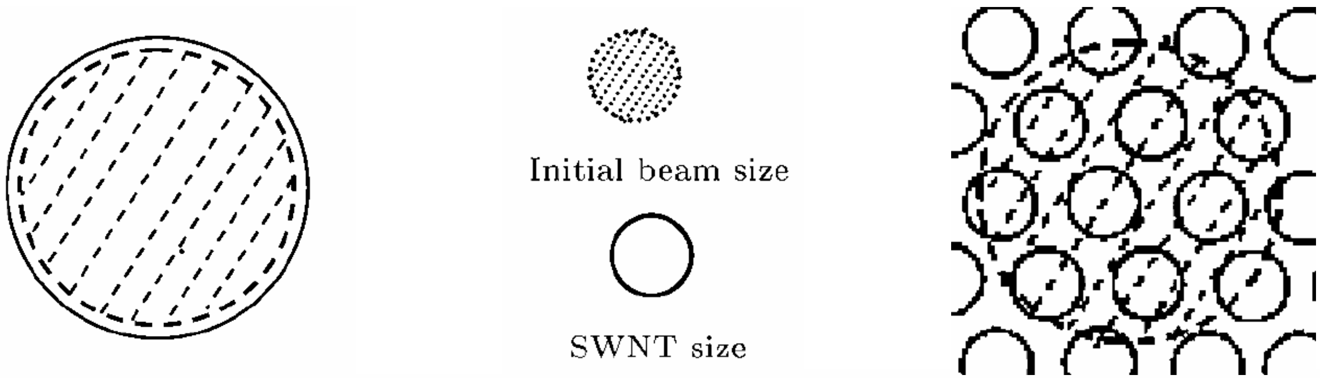
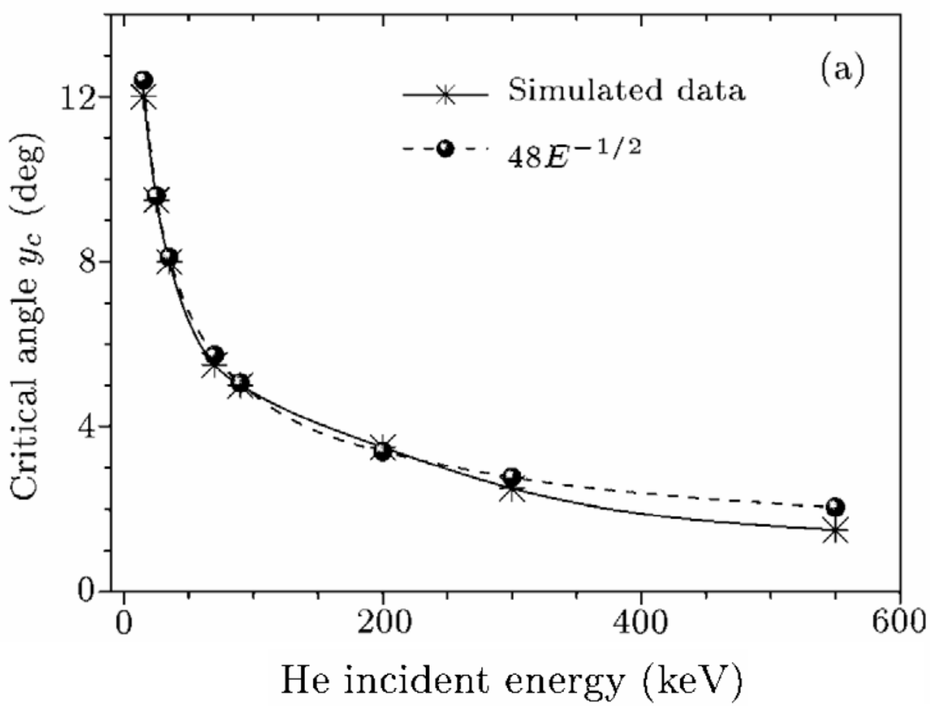
Molecular Dynamics (MD) simulations of ion channeling through carbon nanotubes

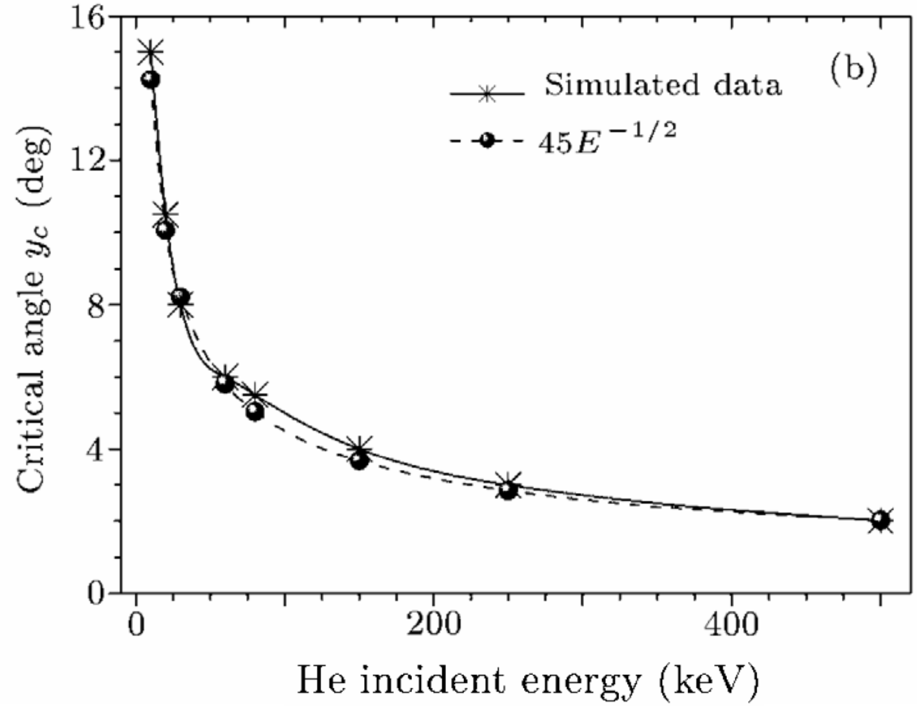
- ❑ Atomistic simulations, solving Newton's equations
- ❑ Low impact energies, nuclear stopping dominates
- ❑ Projectile effectively neutralized near the entrance
- ❑ Empirical potentials (Tersoff/Brenner, van der Waals, and ZBL or Lennard-Jones), truncation issues, charging …
- ❑ Ab-initio (DFT) potentials, 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

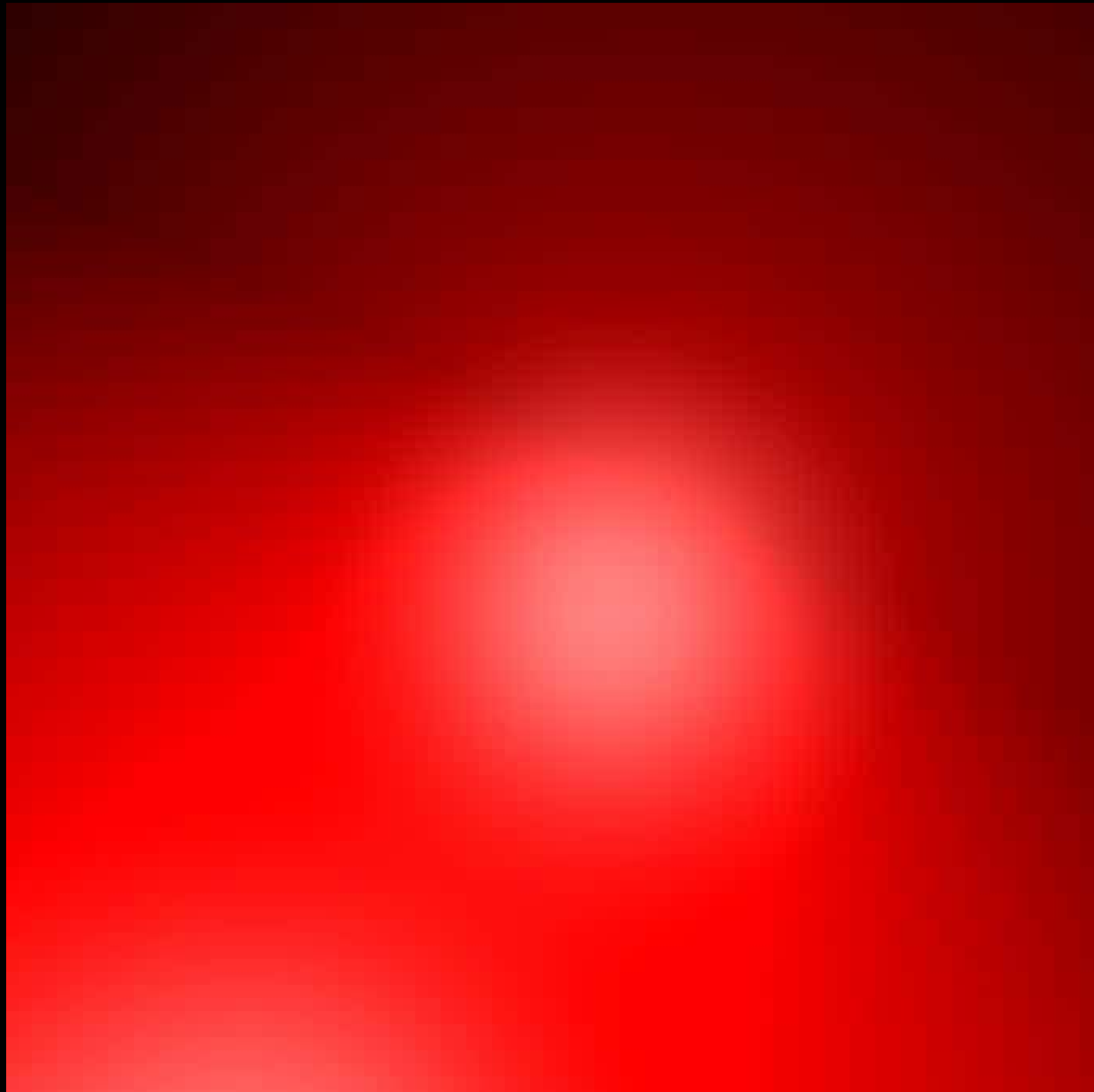
MC sim. of channelling of ~100 keV He^+ ions in a (17,0) SWNT and in rope of (17,0) SWNTs

L.-P. Zheng *et al., Chin. Phys. Lett.* 23 (2006) 2169



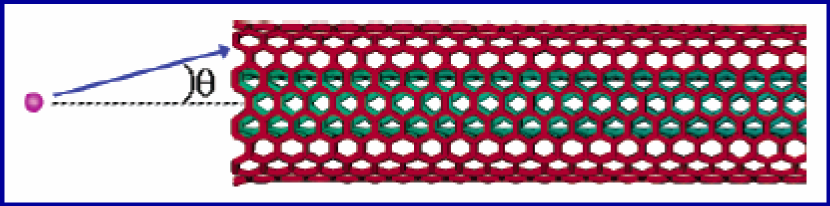






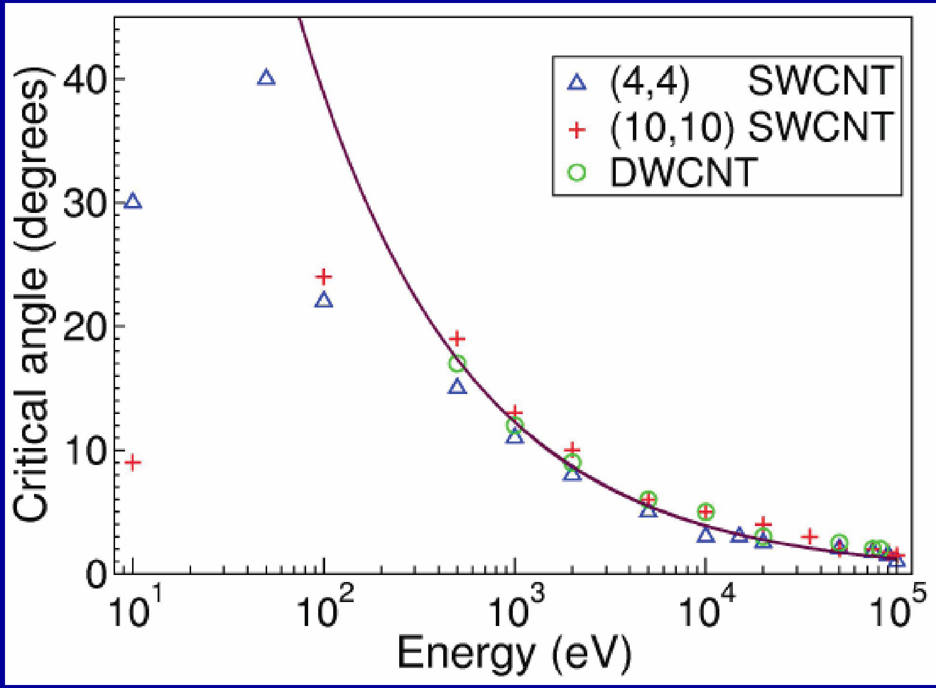
MD sim. of channelling of C^+ ions in SWNT & DWNT

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

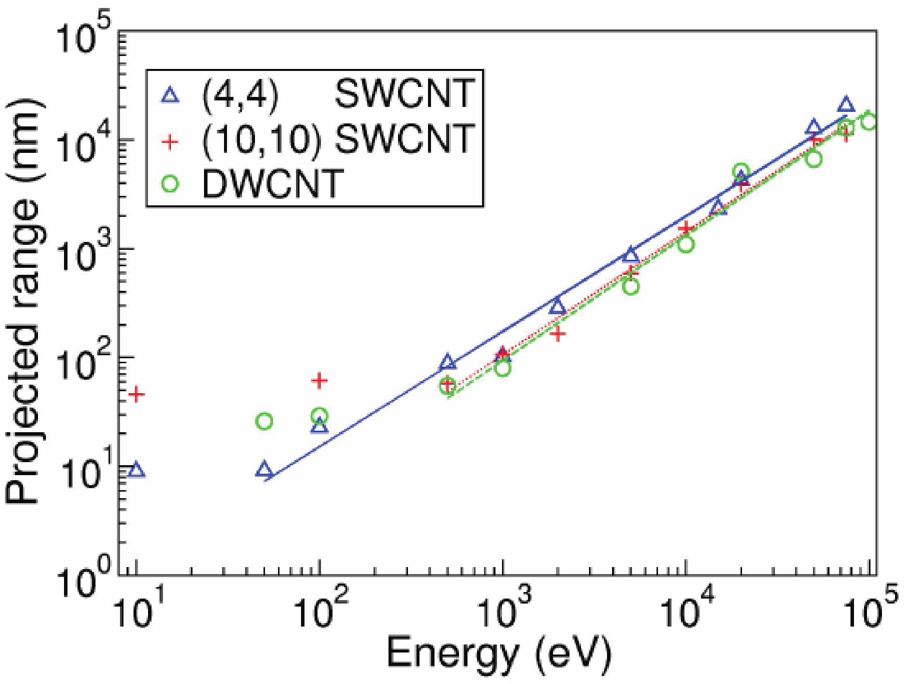


Tersoff potential for C-C in the walls
ZBL potential for projectile - target

Critical angle vs incident energy

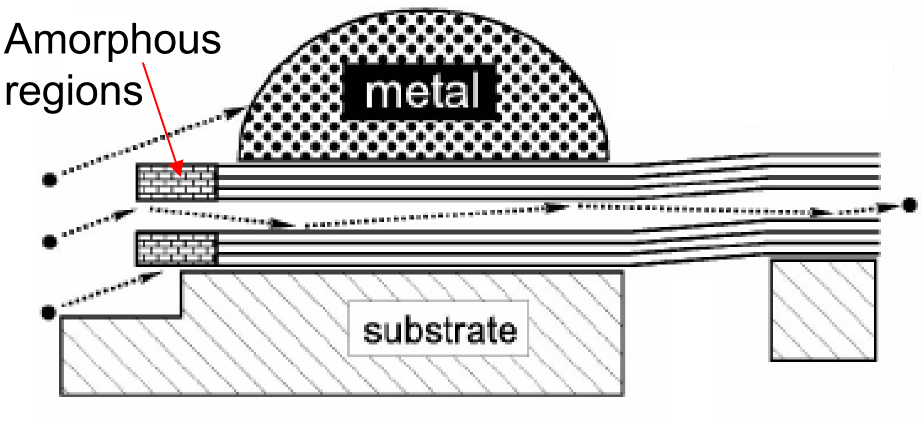


Range vs incident energy



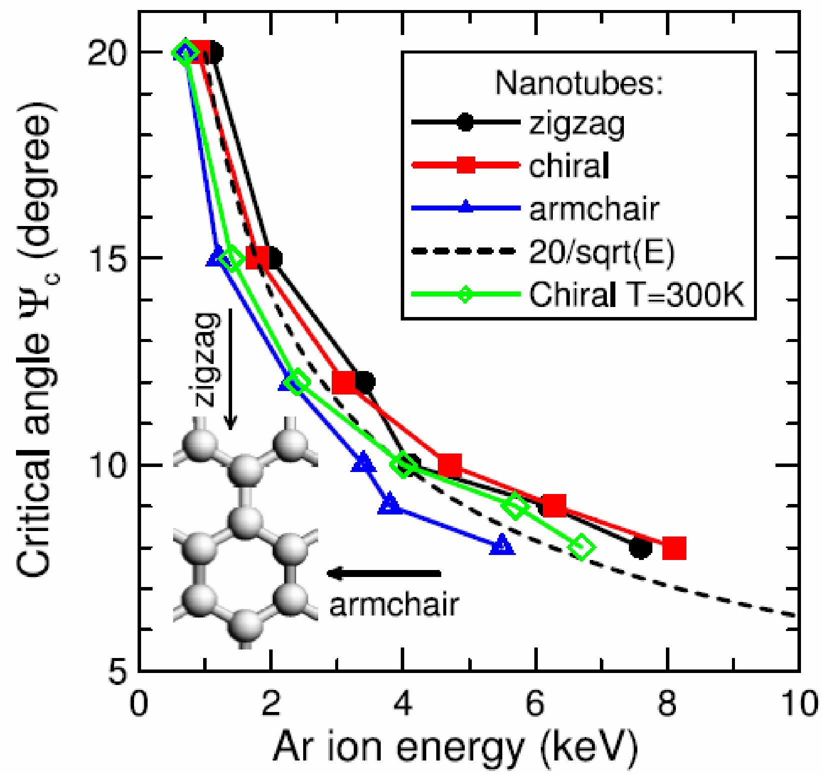
MD sim. of channelling of keV Ar^+ ions in MWNT

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



Critical angle for channelling agrees with continuum model

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



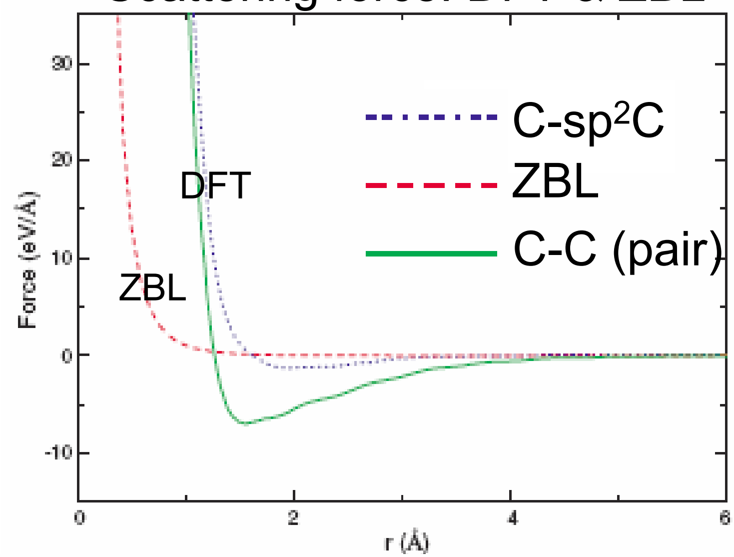
Conclusions:

- channelling dominated by nuclear energy loss (50-100 eV per collision)
- channelling possible even at low energies and large angles (~ 10^o)
- 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

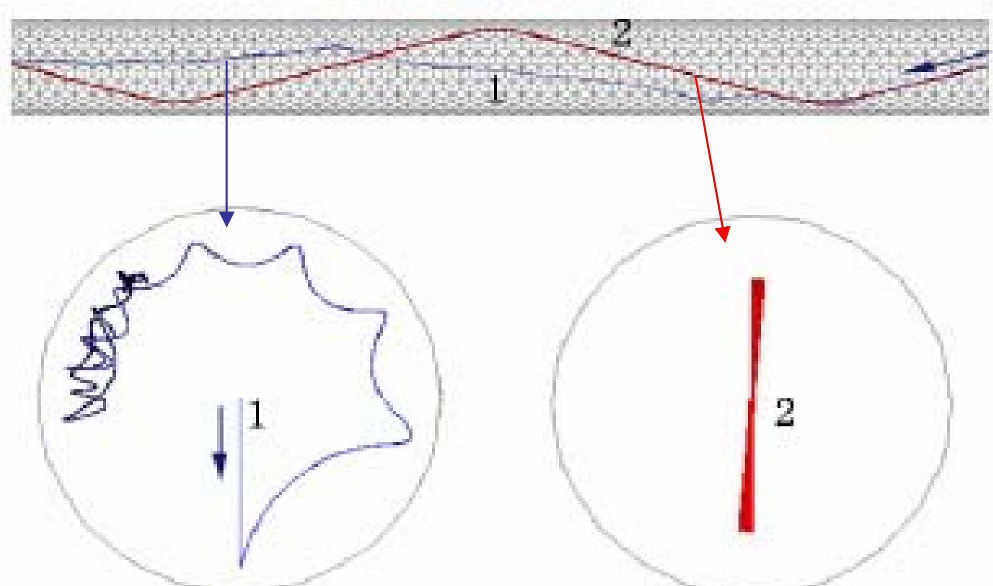
MD sim. of channelling of ~100eV C^+ ions in SWNT

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

Scattering force: DFT & ZBL

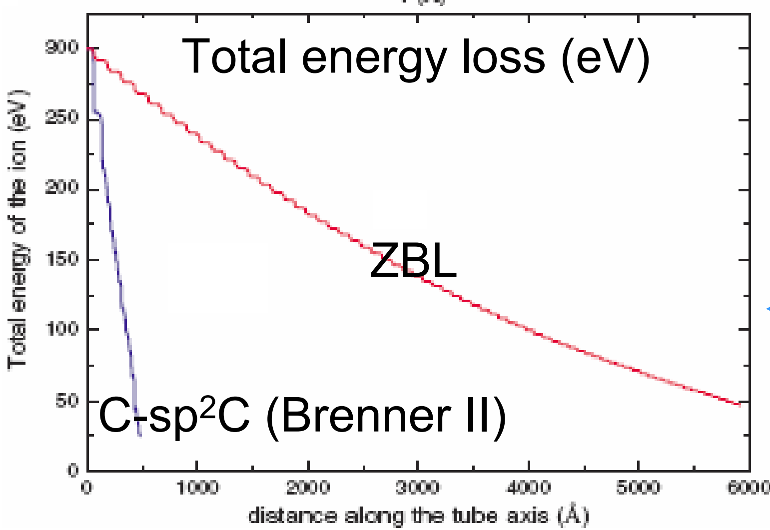


Trajectories for: 1) C-sp^{2}C, 2) ZBL



C-sp^{2}C at 100 eV

ZBL at 100 eV



Electronic energy loss modeled by:
- modified Firsov
- Brandt-Kitagawa

ZBL at 300 eV

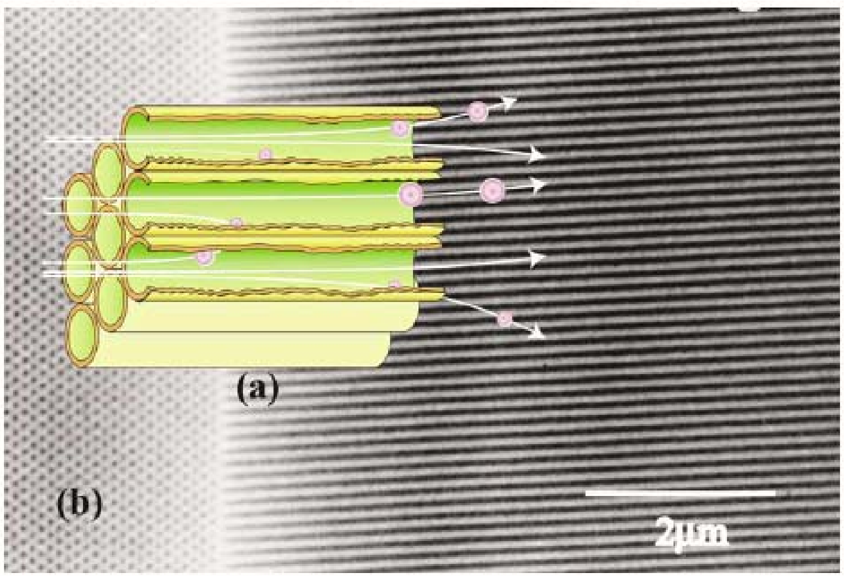
Outline

- **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**

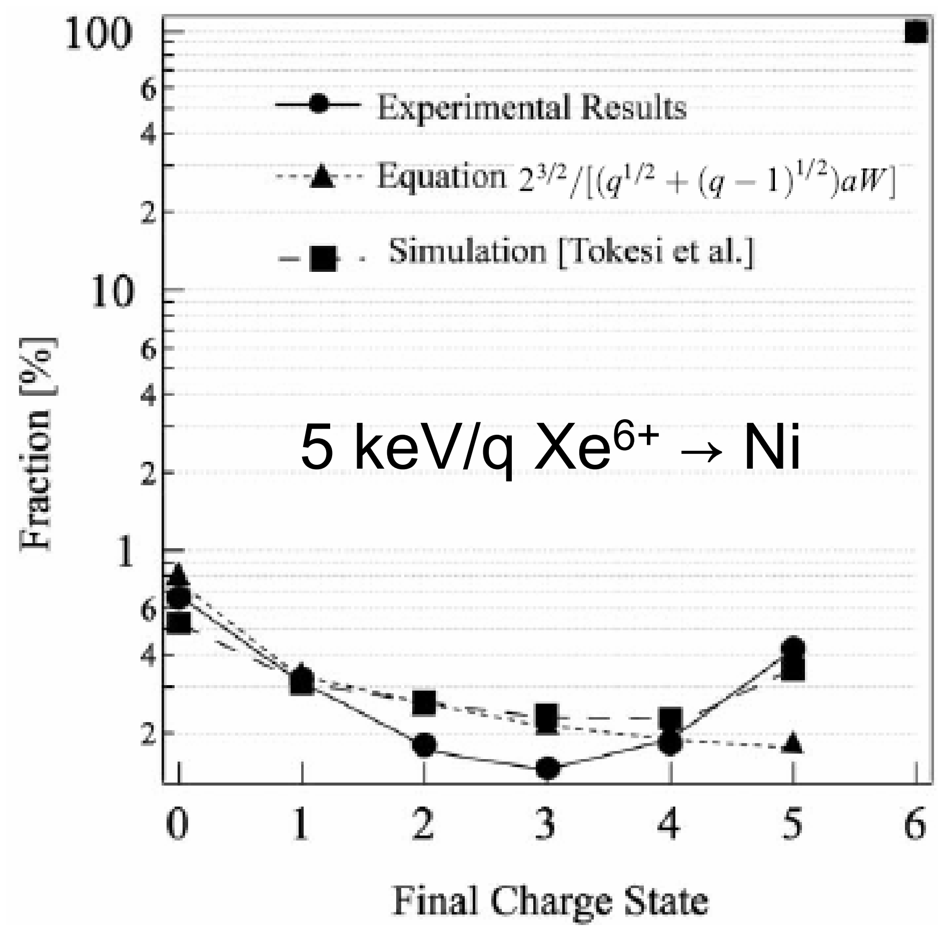
Transmission of highly-charged ions through arrays of metallic capillaries with diamater ~ 100 nm

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 diamater ~ 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

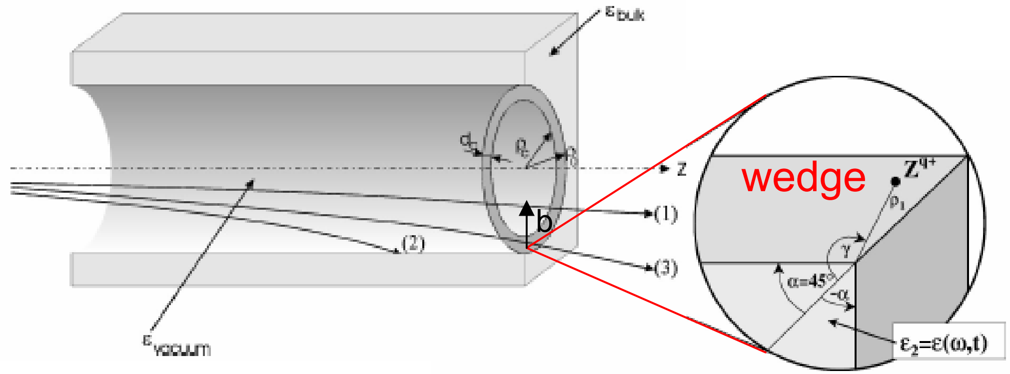
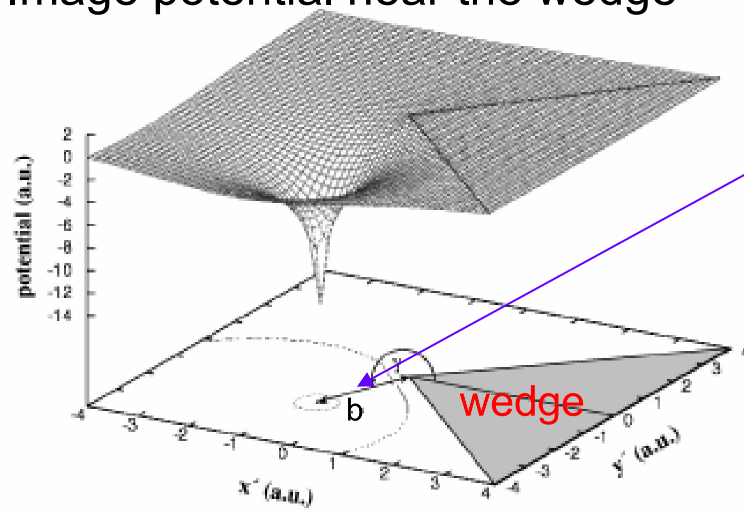
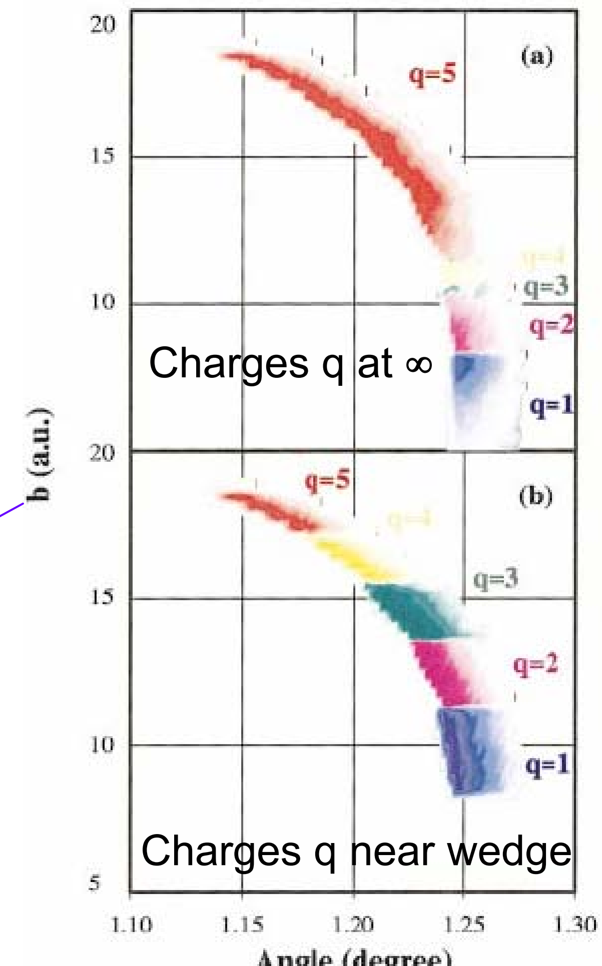


Image potential near the wedge

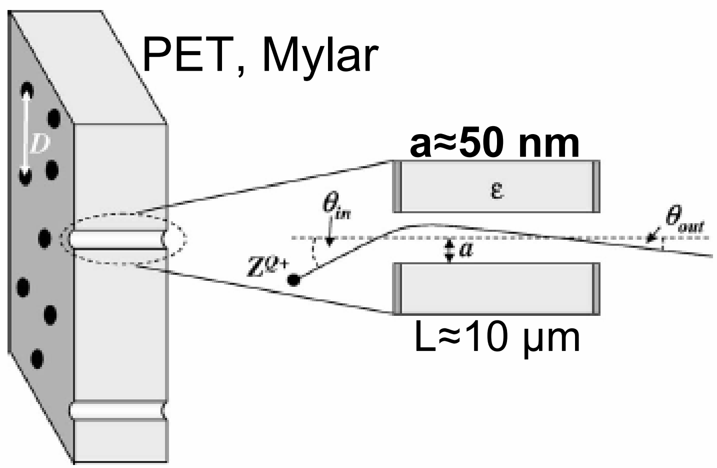


Distributions of 2 keV $N^{6+} \rightarrow Ni$ vs closest dist. b and scattering angle

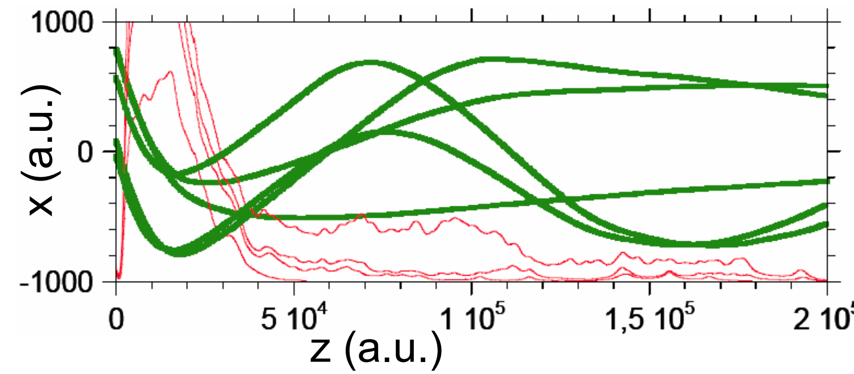


Guiding keV Ne^{7+} ions through insulating capillaries

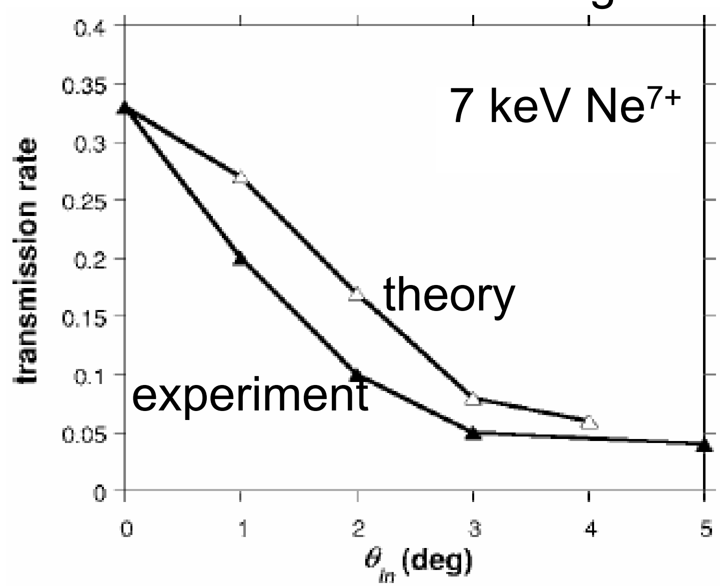
experiment: Gy. Vikor *et al., Nucl. Instr. Meth*. B 233 (2005) 632;
theory: K. Schiessl *et al., Phys. Rev.* A 72 (2005) 62902



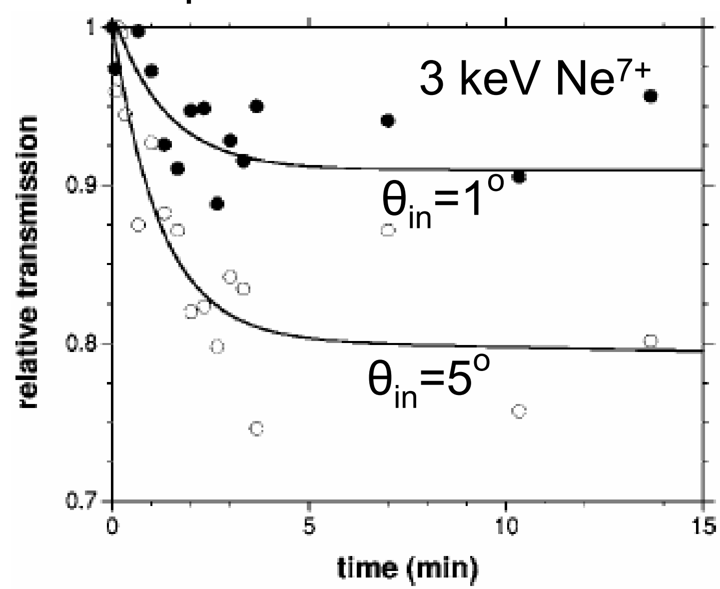
Ion trajectories & deposited charge density



Transmission vs angle



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, dechanneling, projectile charge, entrance/exit 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