Channeling of protons in radially compressed chiral carbon nanotubes

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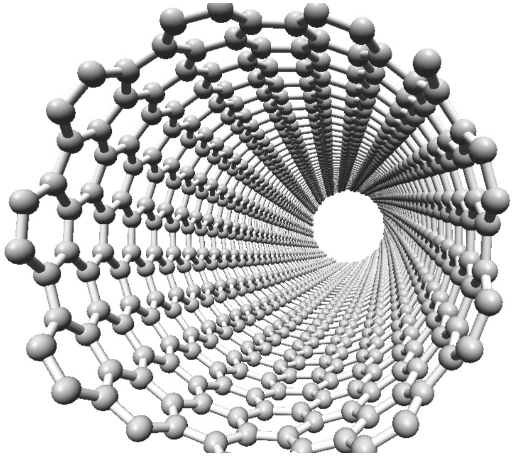


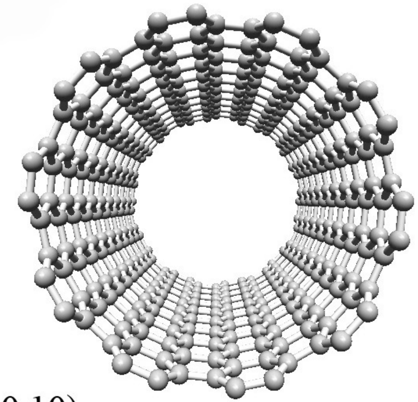
OUTLINE

- Carbon Nanotubes (CNTs)
- Channeling in CNTs
- Motivation
- Simulation model
- Results
- Conclusions
- Future prospects

CARBON NANOTUBES (CNTs) (1/3)

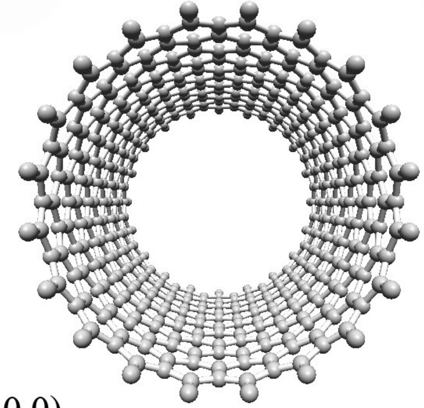
- Types of single-wall nanotubes (SWNTs)

Armchair



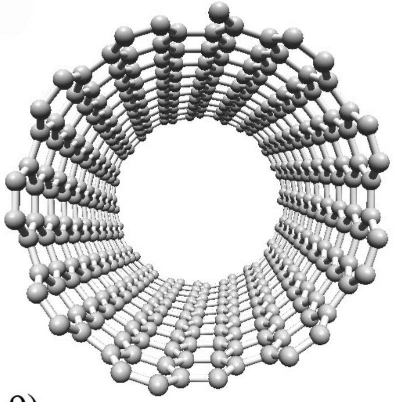
(10,10)

Zig-zag



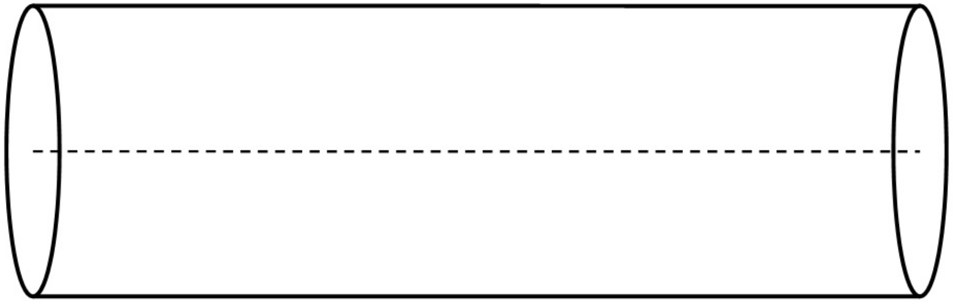
(20,0)

Chiral



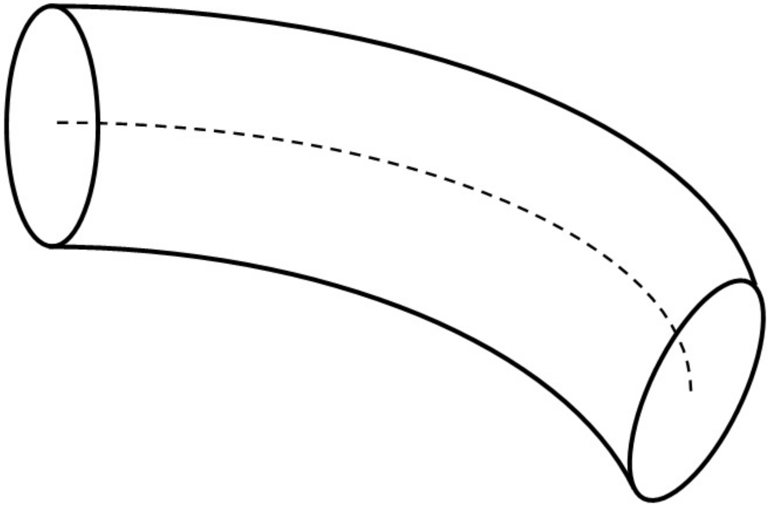
(11,9)

- Straight CNT

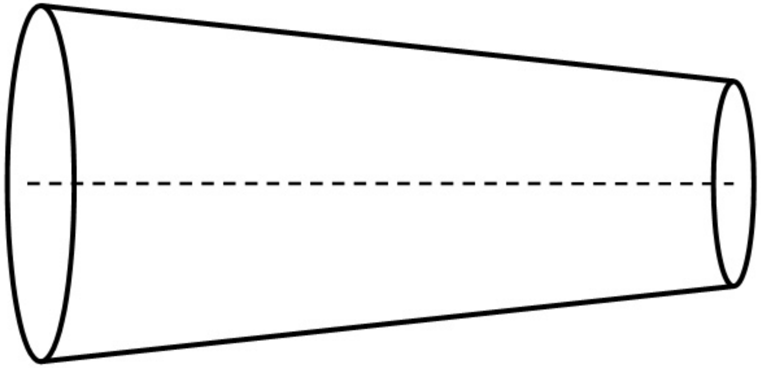


CARBON NANOTUBES (CNTs) (2/3)

- Bent CNT

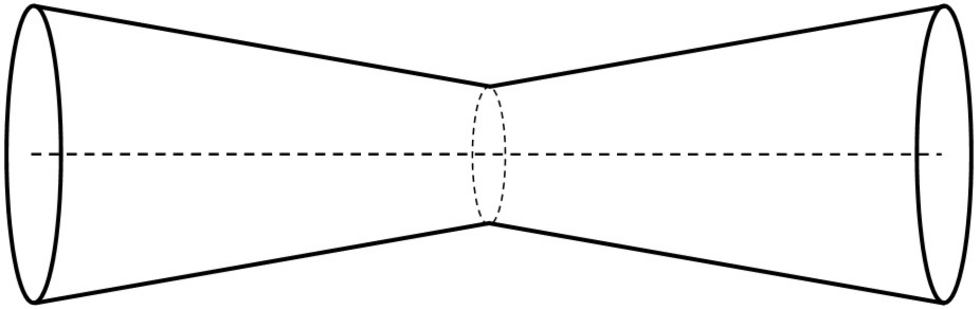


- Radially compressed CNT (at one end)

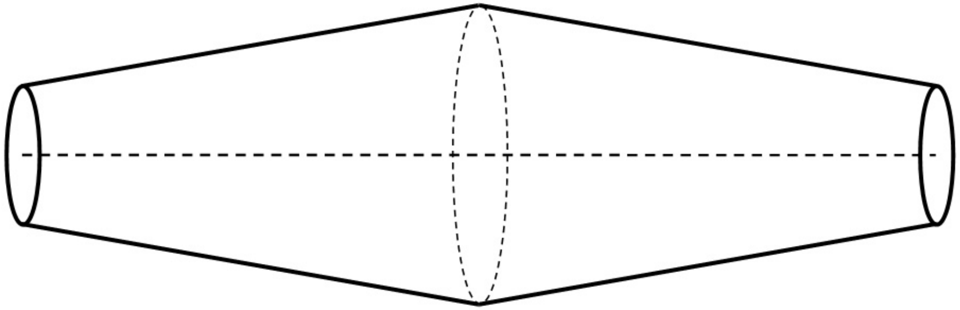


CARBON NANOTUBES (CNTs) (3/3)

- Radially compressed CNT (at the centre)



- Radially compressed CNT (at both ends)



CHANNELING IN NANOTUBES

- Straight & bent CNTs
  (N.K. Zhevago, N.F. Shul' ga, K.A. Ispirian, S.B. Dabagov, X. Artru and others)
- Radially compressed CNTs
  (A. Karabarbounis, S. Sarros, Ch. Trikalinos)
- CNTs with random curvature
  (A.S. Sabirov)

MOTIVATION

- Channeling of charged particles in carbon nanotubes with ideal structure has been investigated thoroughly
- Real carbon nanotubes have structure that differs from ideal
- There is a need for investigation of propagation and channeling of charged particles in carbon nanotubes with more realistic structure

SIMULATION MODEL (1/5)

- Potential of a chiral CNT in Doyle-Turner approximation:

$$U(r,\varphi)=3^{-3/2}32\pi Ze^2l^{-2}R\sum_{j=1}^{4}\alpha_j b_j^2\exp\left[-b_j^2(r^2+R^2)\right]I_0(2b_j^2Rr)$$

where:

$Z = 6$ – atomic number of the target atoms, r – distance from nanotube axis and α_j, b_j – dimensional parameters in the Doyle-Turner approximation:

$\{\alpha_j\}=\{3.222,\ 5.270,\ 2.012,\ 0.5499\}\times10^{-4}\ \mathrm{nm}^2$ $\{b_j\}=\{10.330,\ 18.694,\ 37.456,\ 106.88\}\ \mathrm{nm}^{-1}$

$R=R_0\pm z\cdot\tan\varphi$ – nanotube radius at distance z from entrance,

$R_0=\left(l\sqrt{3}/2\pi\right)\sqrt{n^2+nm+m^2}$ – nanotube radius,

$l=0.142\ \mathrm{nm}$ – length of the bond between the carbon atoms

SIMULATION MODEL (2/5)

- Energy losses calculated by phenomenological expression for the local stopping power given by Lindhard:

$$\frac{\Delta E}{\Delta z} = S(E) = \frac{4\pi Z_1^2 e^4 Z_{val}}{m\upsilon^2}\left[(1-\alpha)+\alpha n_e(r)\right]\ln\left(\frac{2m\upsilon^2}{I}\right)$$

where: $Z_1 e$ and υ – the ion charge and velocity respectively, α – part of close collisions ($\alpha = 0.5$), Z_{val} – number of valence electrons per atom,
m – electron mass, $I = I_0 Z$ – average excitation potential ($I_0 \cong 13.5$ eV,
Z – atomic number of target atoms)

$$n_e(r) = \frac{2NZ_{val}}{\pi d_R}\sum_{j=1}^{5}\alpha_j^{(e)} b_j^{(e)2} \exp\left[-b_j^{(e)2}(R^2+r^2)\right] I_0(2b_j^{(e)}Rr)$$

- Equations of motion calculated from Newton's second law as:

$$m_1\frac{d^2\boldsymbol{r}}{dt^2} = -\left(\frac{\partial U(x,y,z)}{\partial x}\hat{\boldsymbol{i}} + \frac{\partial U(x,y,z)}{\partial y}\hat{\boldsymbol{j}}\right)$$ (m_1 – proton mass)

SIMULATION MODEL (3/5)

- Electronic multiple scattering is taken into account after each integration step, calculating a normal distribution of the scattering angle with standard deviation:

$$\theta_{ms}^2 = \frac{m\Delta E}{2m_1 E}$$

(E and ΔE – the energy and the energy loss at each integration step, respectively)

- Initial conditions:
- beam angle of incidence = 0
- beam well collimated ($\Delta\theta = 0$)
- beam energy spread = 0 (E = 10 MeV)

- Dechanneling of protons:

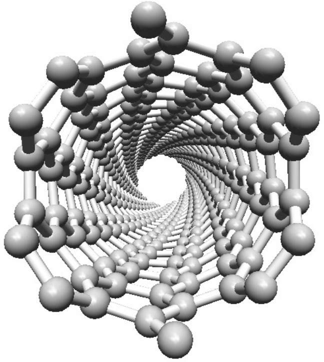
when protons approach CNT walls at distance: $r \le r_c$

($r_c = \sqrt{2}u_\perp$, $u_\perp = 8.5 \cdot 10^{-3}\ nm$)

SIMULATION MODEL (4/5)

- Carbon nanotube types used:

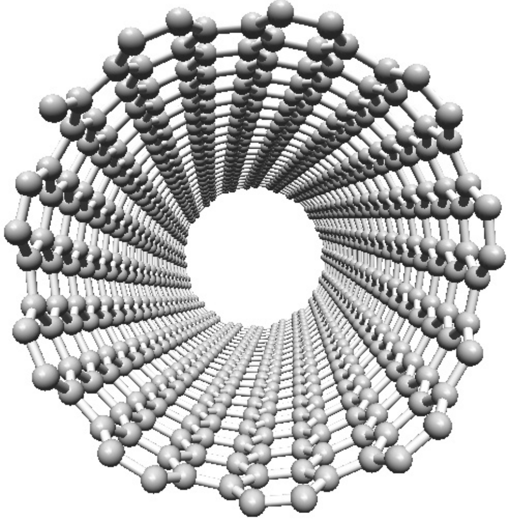
  - **(6,4):**



$$R = 0,341\ nm$$

$$\psi_{cr} = 2,181\ mrad \quad (\text{at } E = 10\ MeV)$$

  - **(11,9):**

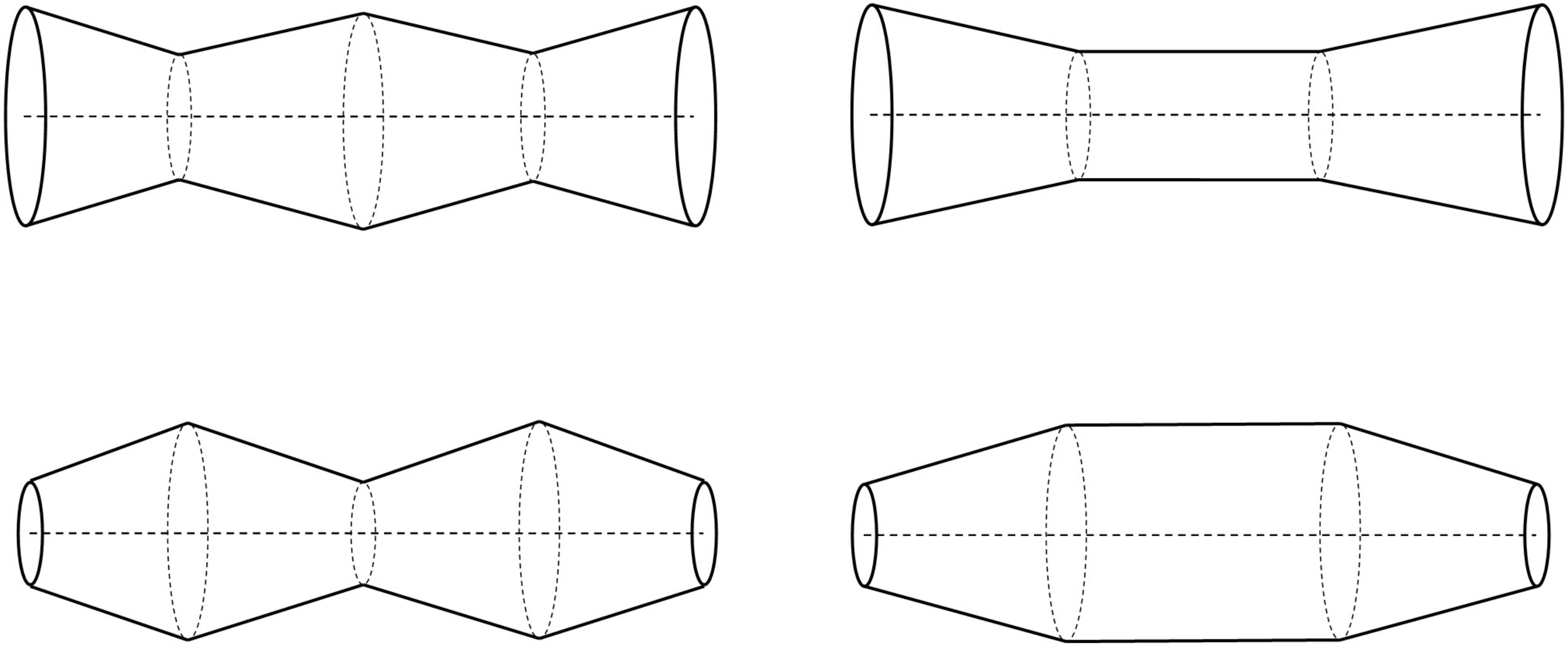


$$R = 0,679\ nm$$

$$\psi_{cr} = 2,169\ mrad \quad (\text{at } E = 10\ MeV)$$

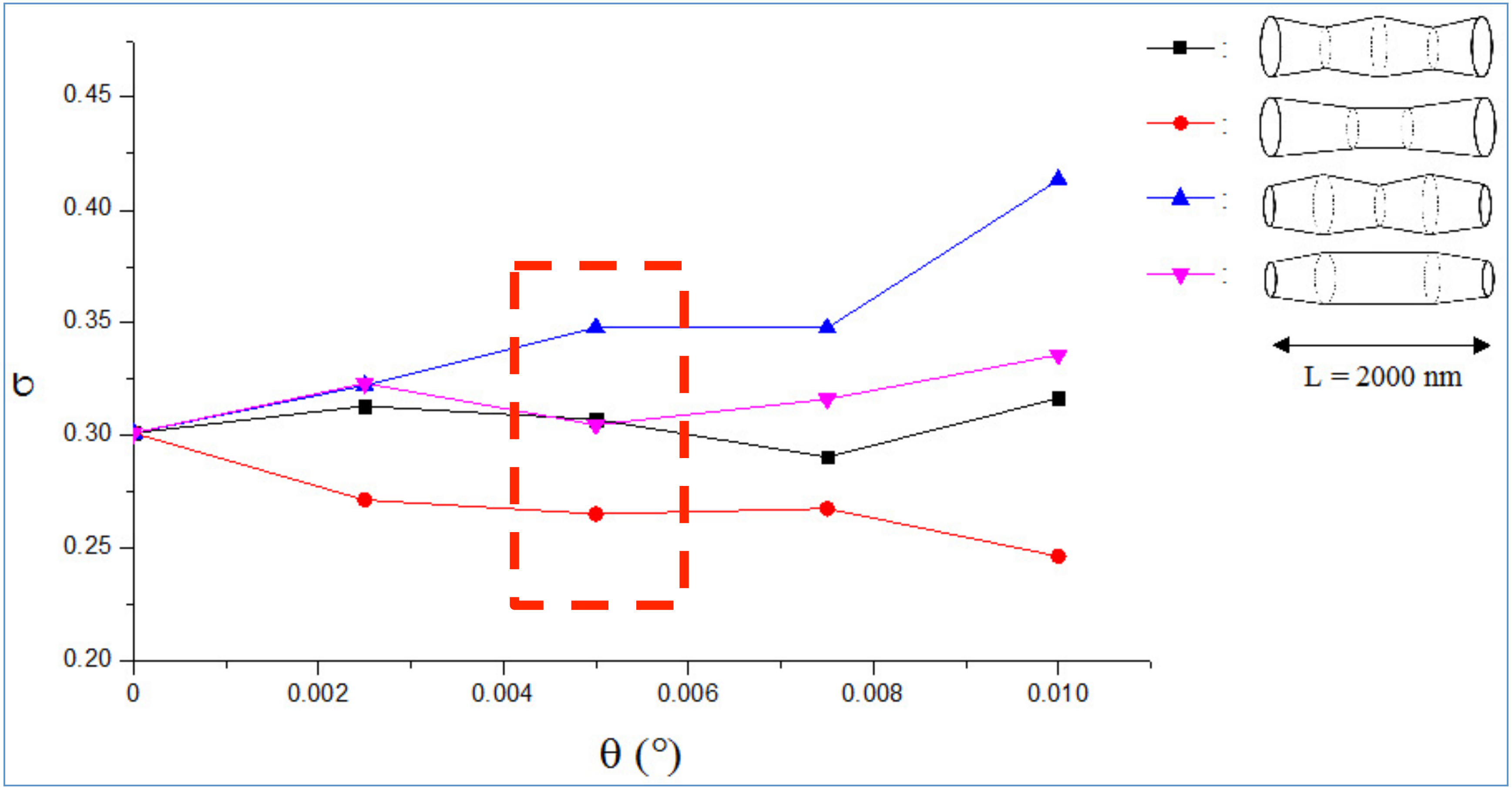
SIMULATION MODEL (5/5)

- Types of radially compressed carbon nanotubes used:



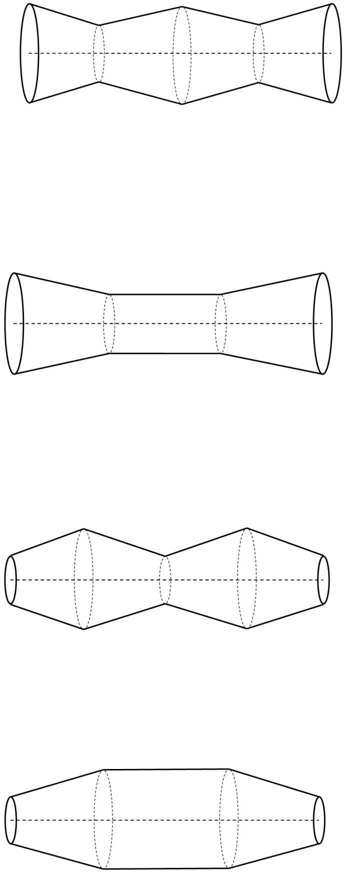
RESULTS (1/6)

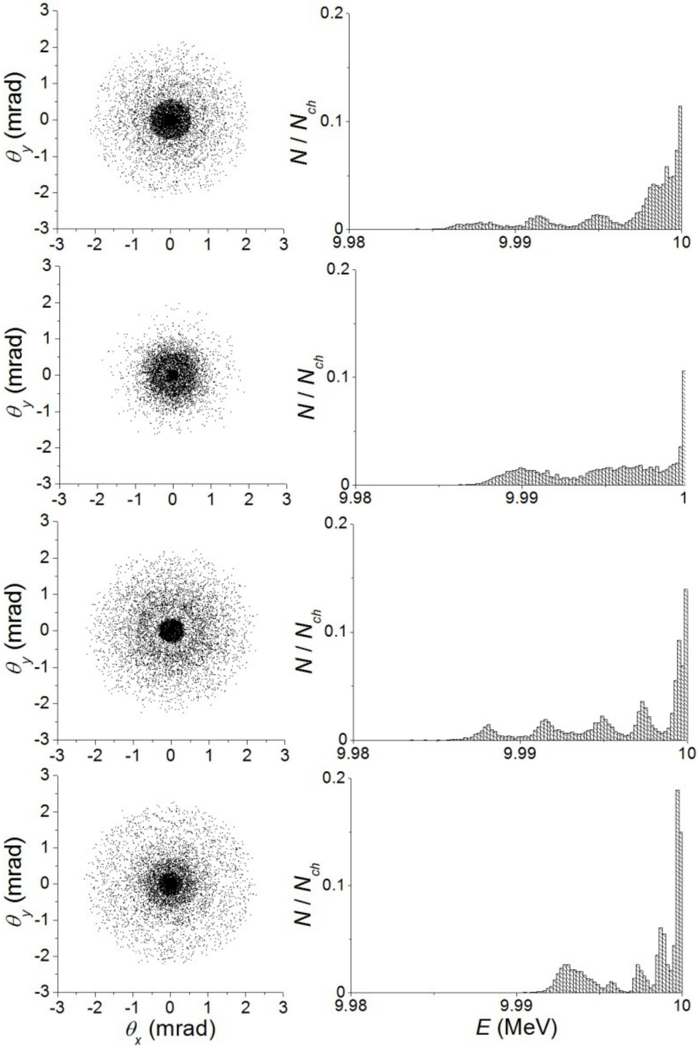
Standard deviation of angular distribution (θ_x section) vs. angle θ of wall slope of compressed CNTs **(6,4)**



RESULTS (2/6)

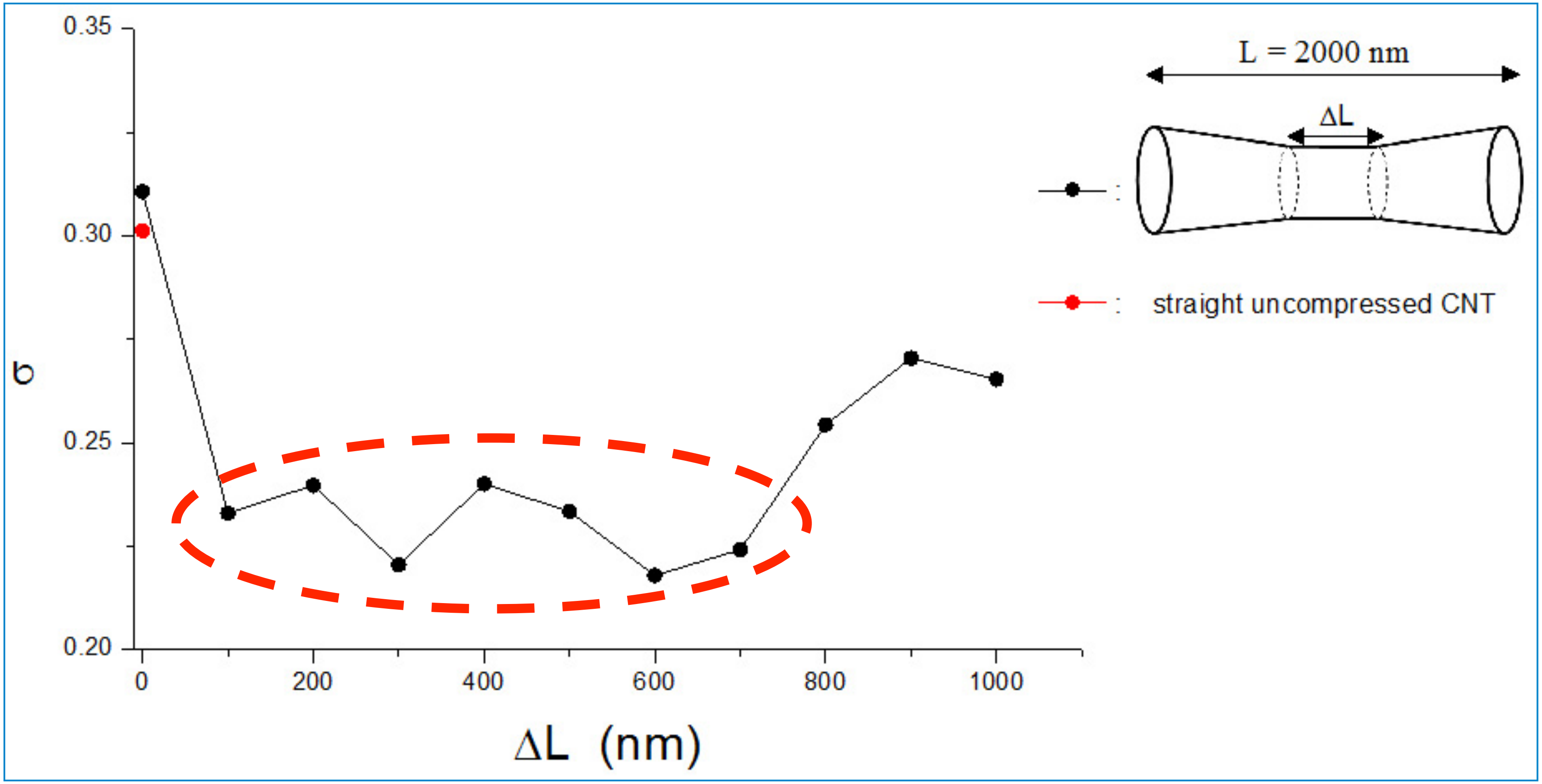
Angular and energy distribution - compressed CNTs **(6,4)** ($\theta = 0.005°$)





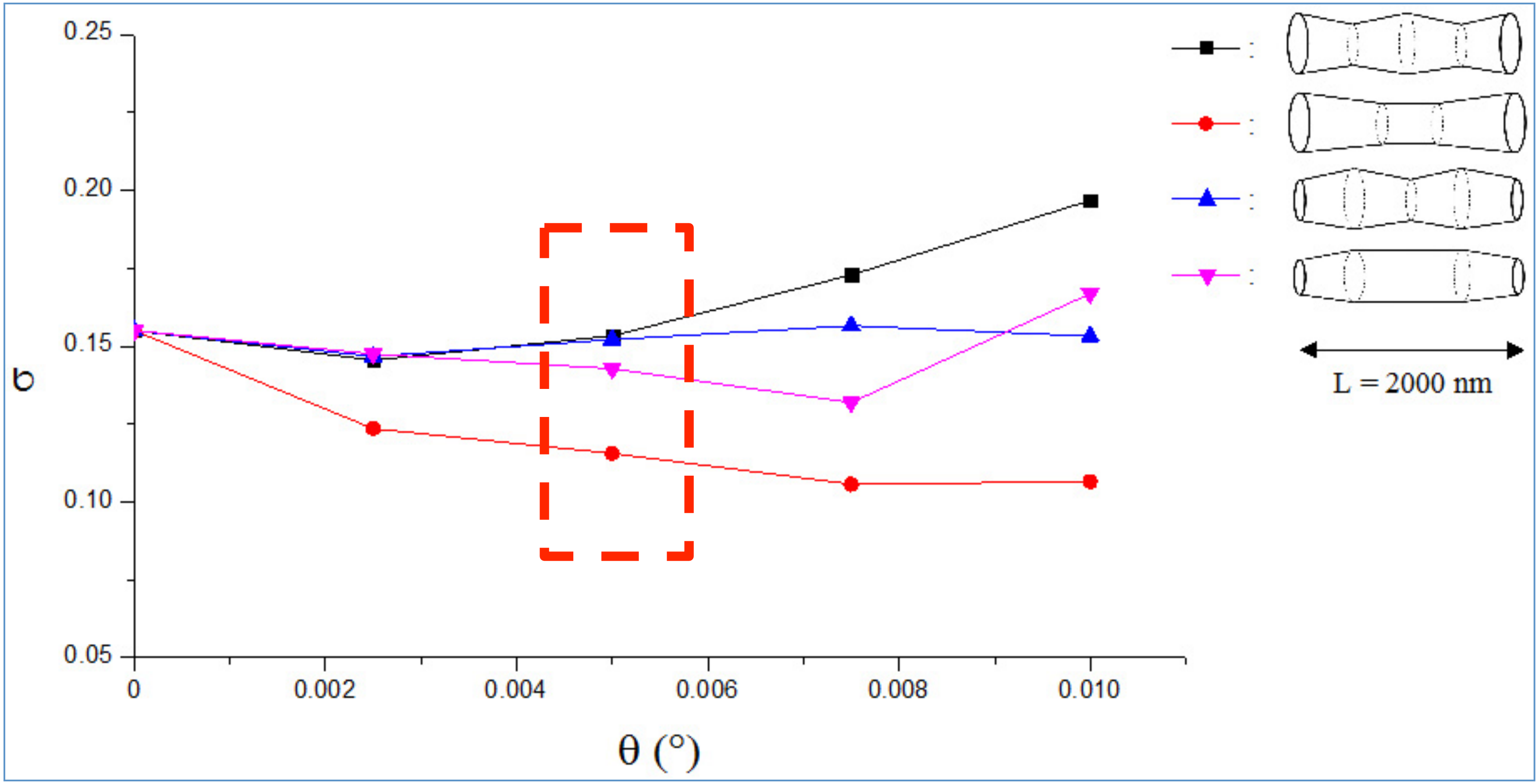
RESULTS (3/6)

Standard deviation of angular distribution (θ_x section) vs. angle θ of wall slope of compressed CNTs **(6,4)**



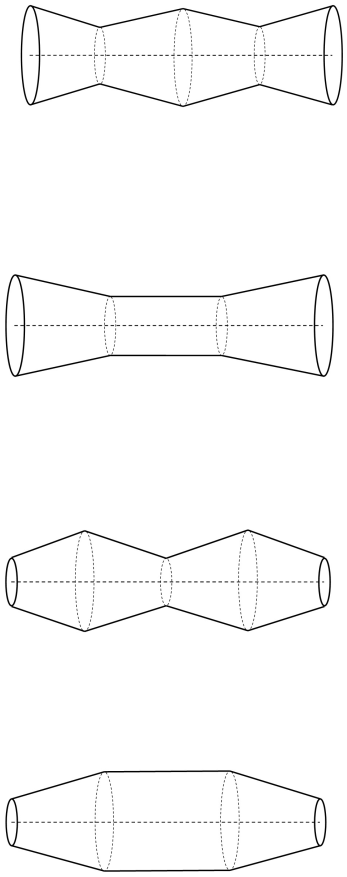
RESULTS (4/6)

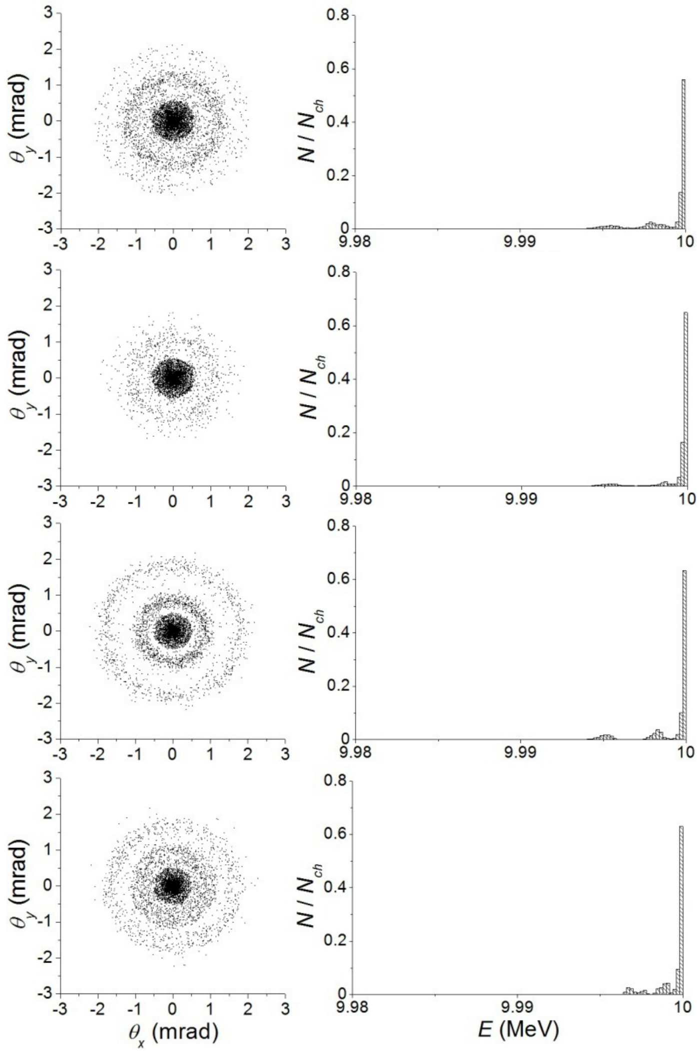
Standard deviation of angular distribution (θ_x section) vs. angle θ of wall slope of compressed CNTs **(11,9)**



RESULTS (5/6)

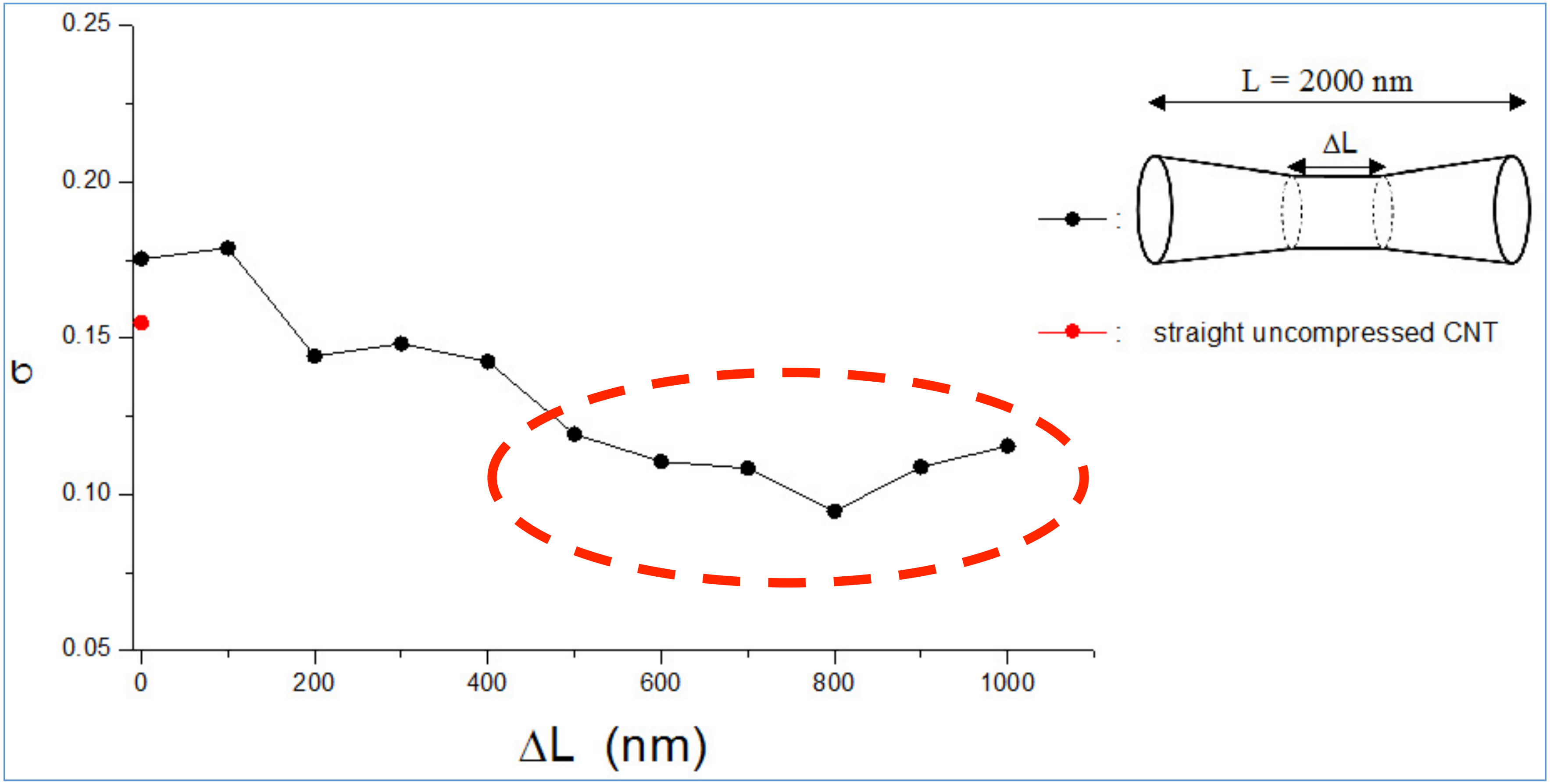
Angular and energy distribution - compressed CNTs **(11,9)** (θ = 0.005°)





RESULTS (6/6)

Standard deviation of angular distribution (θ_x section) vs. angle θ of wall slope of compressed CNTs **(11,9)**



CONCLUSIONS

- Divergence from ideal structure of CNTs could be positive for beam focusing in some cases

- Some types of radially compressed CNTs show better angular distribution not only from other types, but from straight CNT as well

- Angular and energy distributions depend on angle and type of compression

FUTURE PROSPECTS

- Channeling in radially compressed carbon nanotube bundles
- Channeling at different initial conditions (energy, angle of incidence, beam collimation, beam spread)
- Channeling in other types of compressed carbon nanotubes
- Channeling in bent carbon nanotubes radially compressed at one end

Thank you for your attention!