Channeling of protons in various types of radially compressed carbon nanotubes

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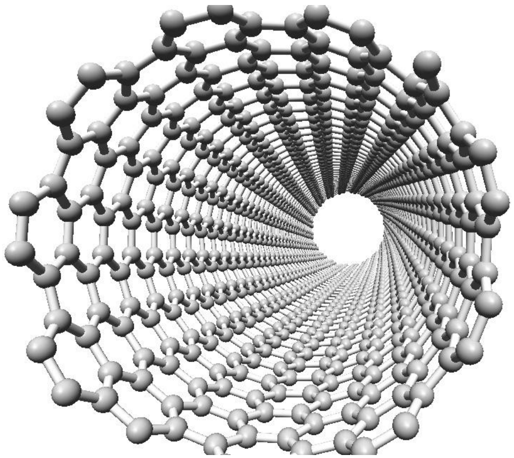


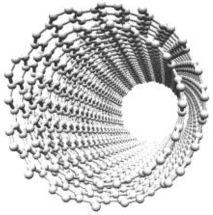
Channeling effect

- Crystals
  - Computer calculations (Robinson et al., 1963)
  - Theoretical description (Lindhard et al., 1965)
  - Experiments (1963 until now)
  - Channeling Radiation (Kumakhov et al., 1976)

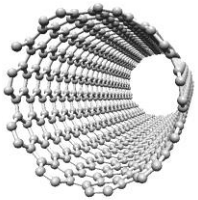
- Carbon Nanotubes (CNTs)
  - Theoretical works (1997 – present)

Carbon Nanotubes

- Discovered
  - 1991 (MWCNT or MWNT)



  - 1993 (SWCNT or SWNT)



- Applications
  - Composite Materials
  - Microelectronics
  - Hydrogen storage
  - High Energy Physics/Channeling (?)

Channeling in carbon nanotubes

- Channeling of charged particles in straight and bent CNTs

  (N.K. Zhevago, N.F. Shul'ga, K.A. Ispirian, X. Artru and others)

- Channeling of x-rays in straight CNTs

  (S.B. Dabagov, N.K. Zhevago and others)

- Channeling of charged particles in radially compressed CNTs

  (A. Karabarbounis, S. Sarros, Ch. Trikalinos)

Channeling of charged particles in straight chiral carbon nanotubes

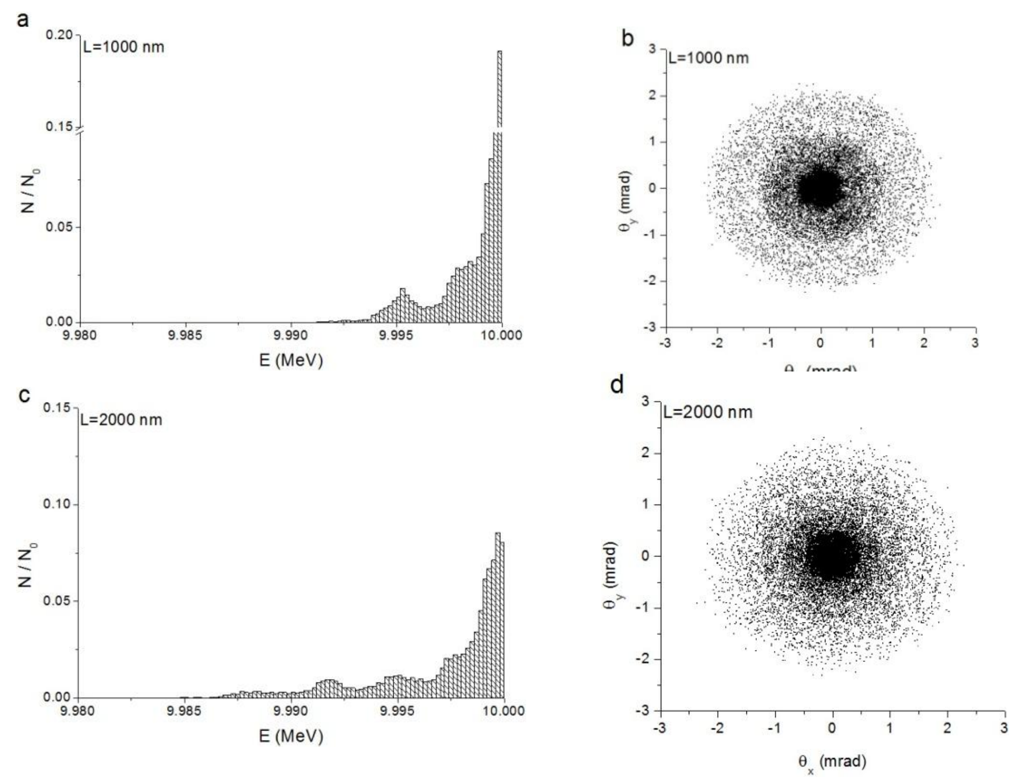
(A. Karabarbounis, S. Sarros, Ch. Trikalinos:

"*Channeling and energy losses of 10 MeV protons in straight chiral carbon nanotube bundles*", NIM B 316 (2013), 160-170)

Straight (6,4) CNT bundle

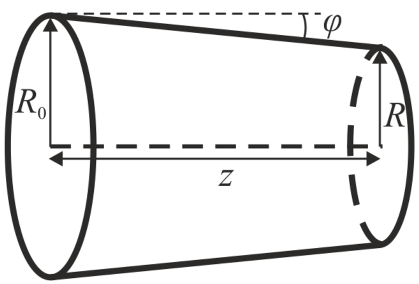
Initial proton energy:
10 MeV

Length of CNT:
1000 nm, 2000 nm



Channeling of charged particles in radially compressed CNTs (compression at one end)

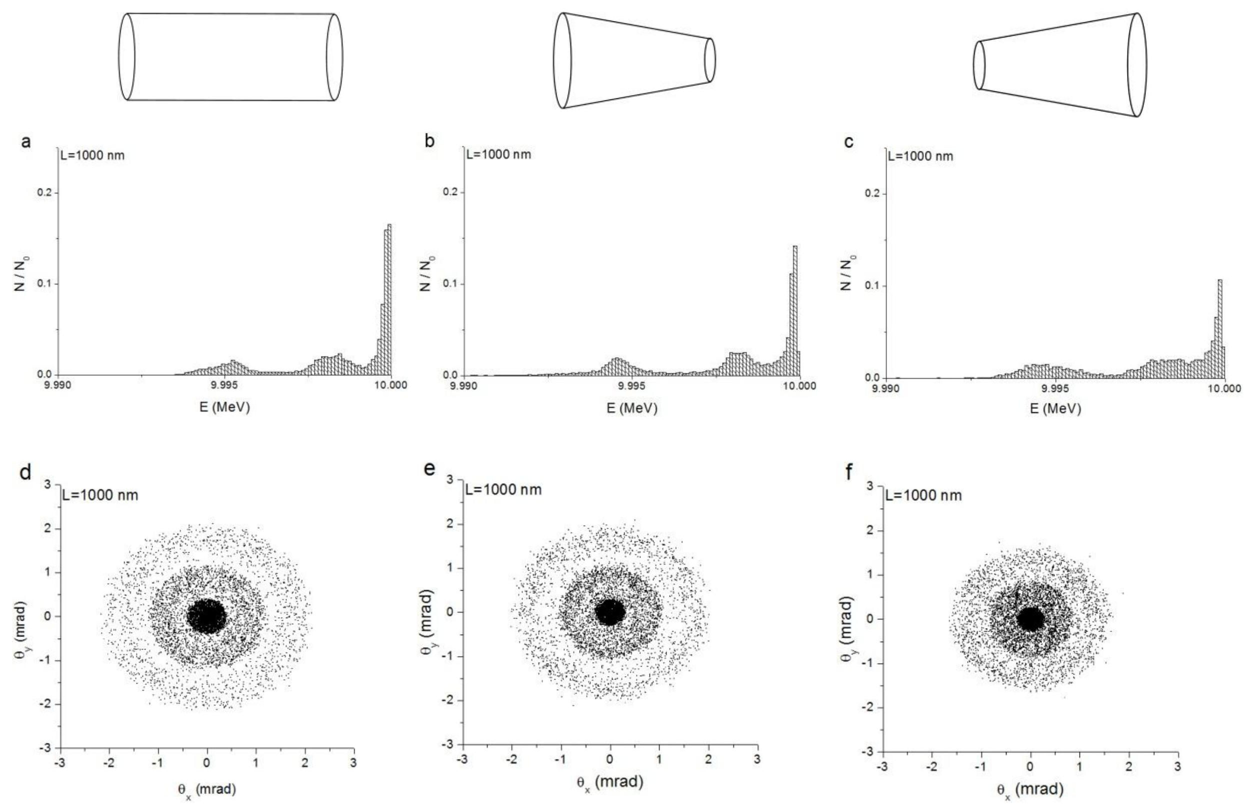
(A. Karabarbounis, S. Sarros, Ch. Trikalinos:
"*Channeling of protons in radially compressed carbon nanotubes*", Journal of Physics: Conference Series 517 (2014) 012038) – Presented at RREPS-2013



$$R = R_0 - z \cdot \tan\varphi$$

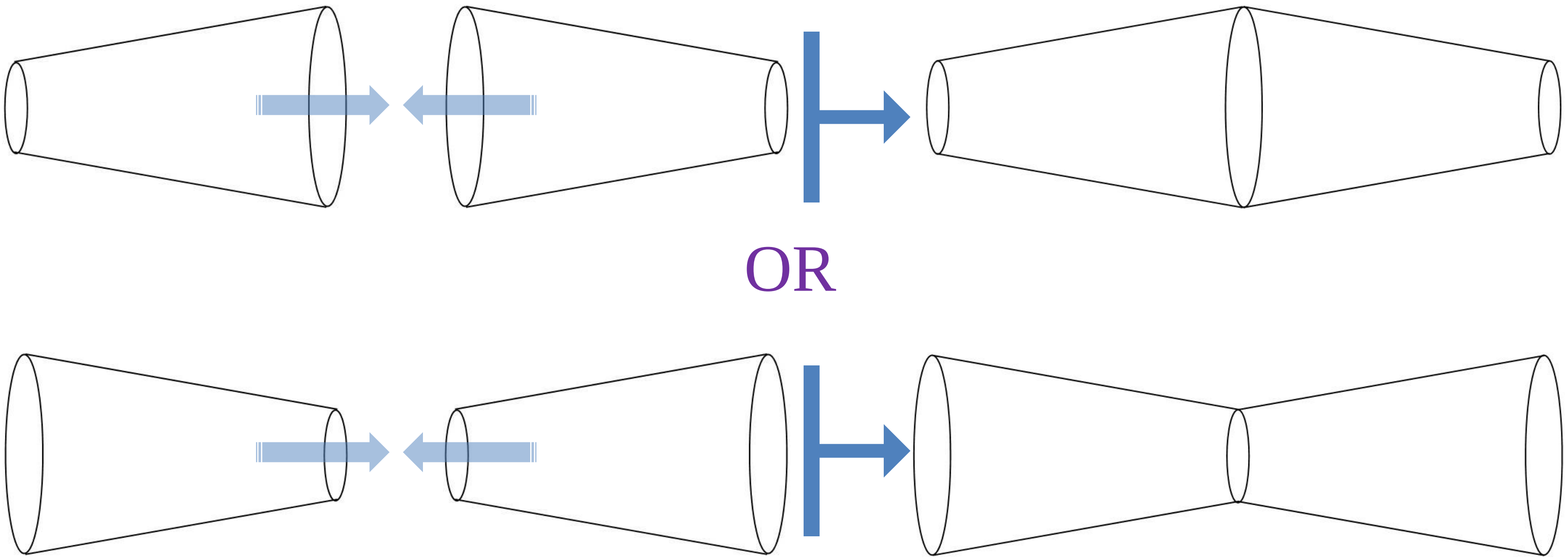
Compressed (6,4) CNT
(φ = 0.005°)
Initial proton energy:
10 MeV

Length of CNT:
1000 nm



Channeling of charged particles in radially compressed CNTs (compression at both ends or at nanotube's centre)

Combining two radially compressed (at one end) CNTs:



Model used for simulation:

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

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

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:

$\{\alpha_j\} = \{3.222,\ 5.270,\ 2.012,\ 0.5499\} \times 10^{-4}\ \text{nm}^2$ $\{b_j\} = \{10.330,\ 18.694,\ 37.456,\ 106.88\}\ \text{nm}^{-1}$

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

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

$l = 0.142$ nm – length of the bond between the carbon atoms

Model used for simulation:

- 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:

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

Model used for simulation:

- 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 incident angle = 0
  - beam well collimated ($\Delta\theta = 0$)
  - beam energy spread = 0 (E = 10MeV)

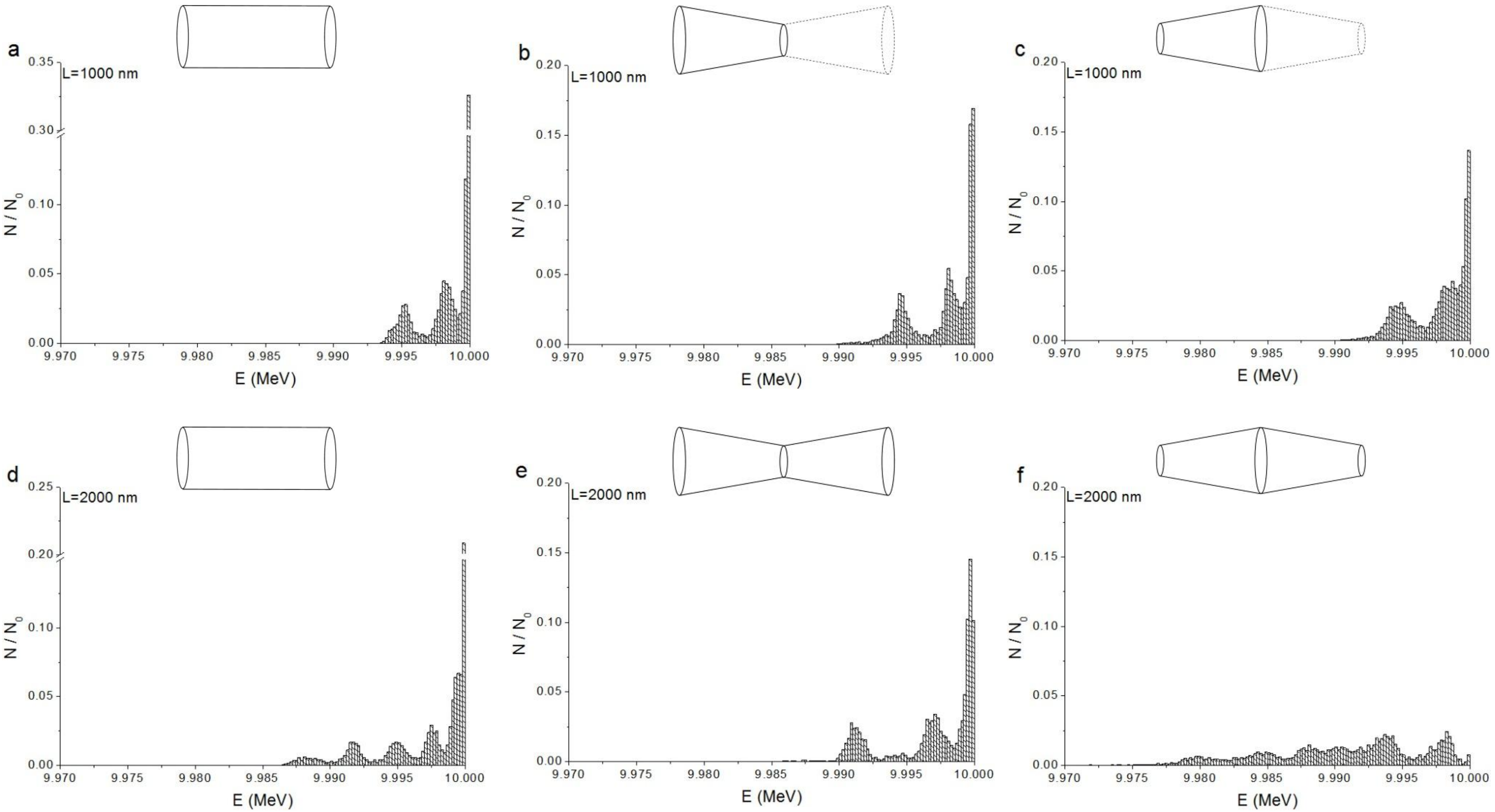
- Dechanneling of protons:

when protons approach CNT's walls at distance: $r \le r_c = \sqrt{2u_\perp}$ $(u_\perp = 8.5 \cdot 10^{-3} nm)$

Comparison between straight and compressed CNTs (6,4) with φ = 0.005°

Energy distribution

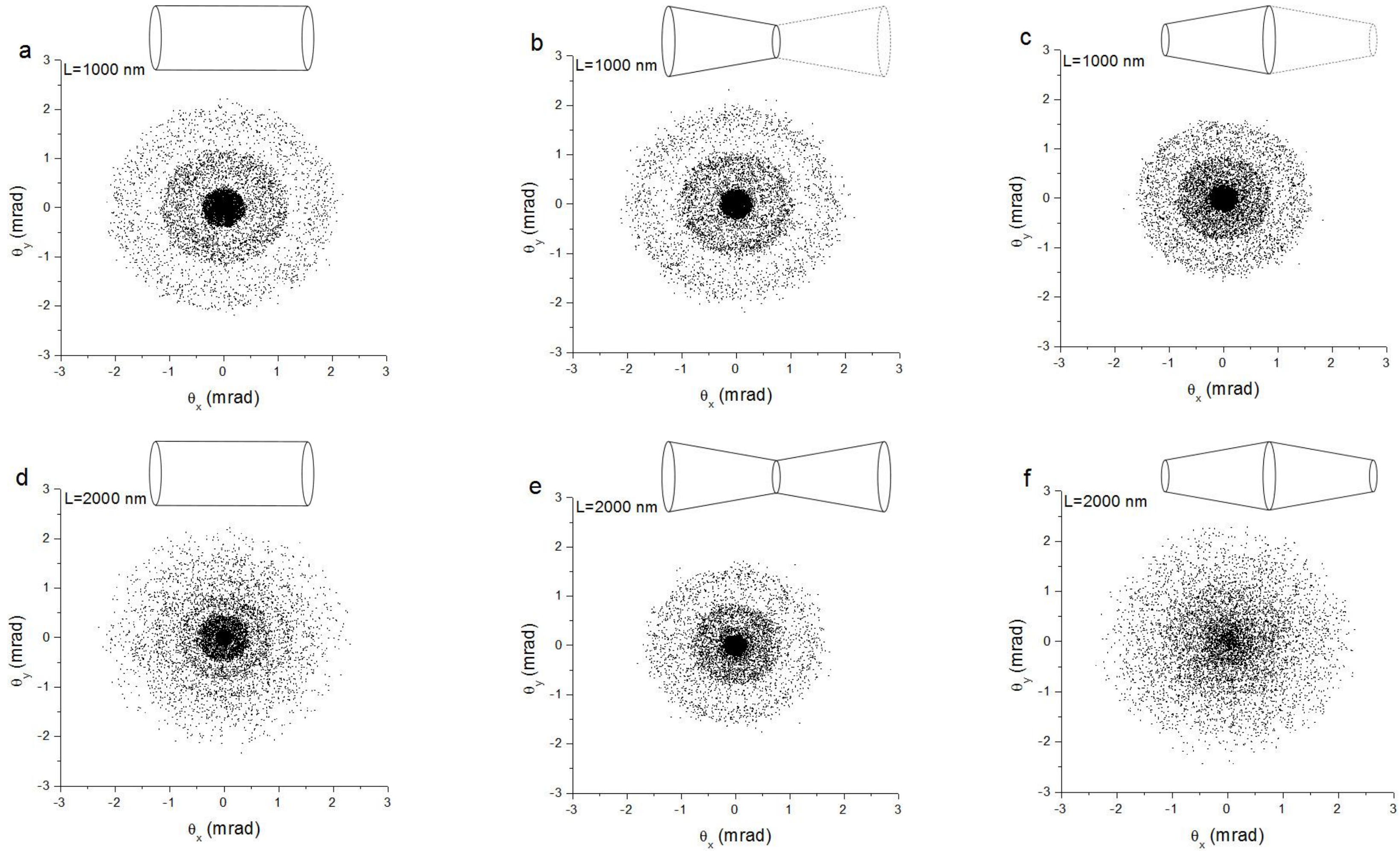
(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Comparison between straight and compressed CNTs (6,4) with φ = 0.005°

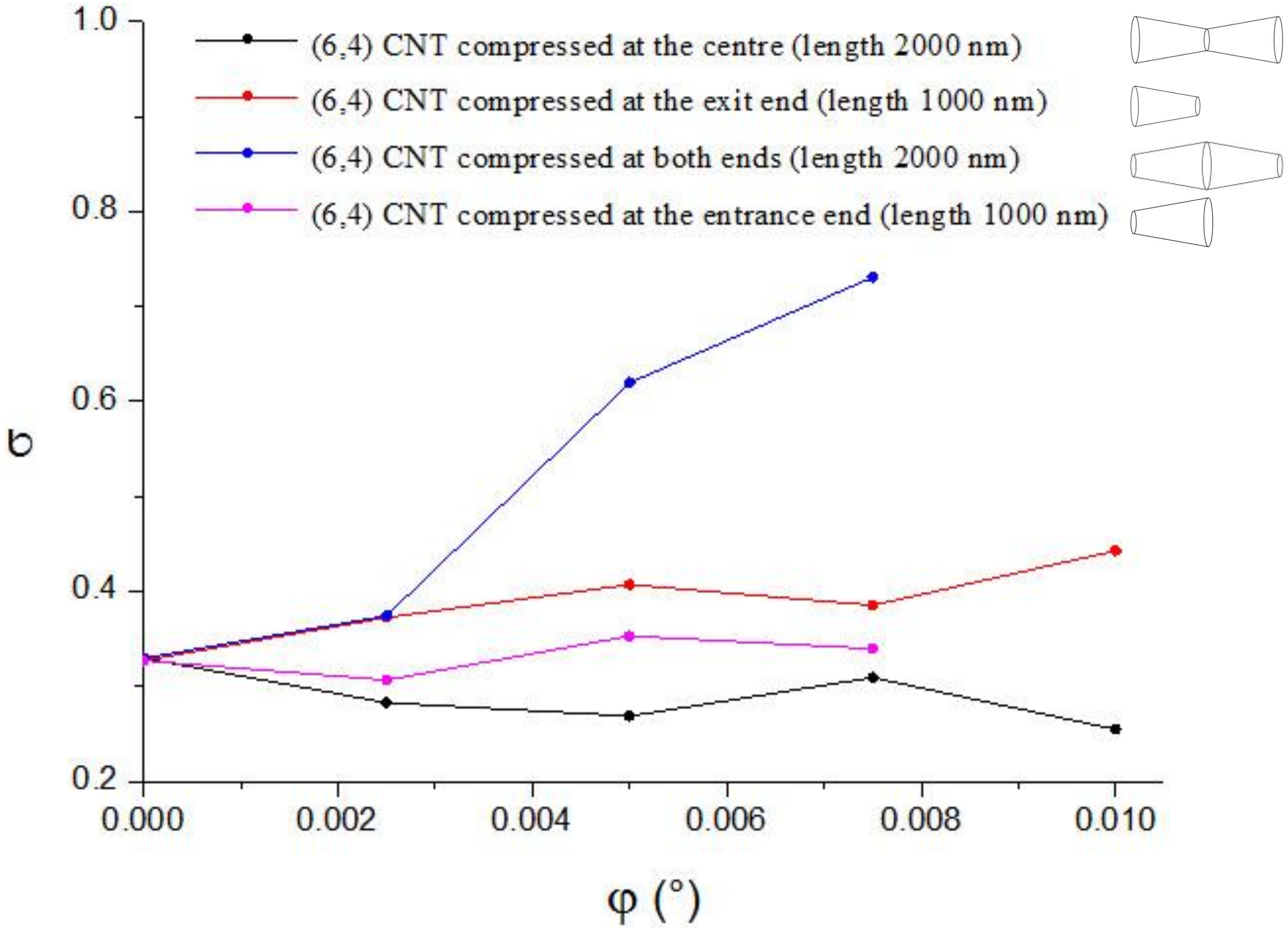
Angular distribution

(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Standard deviation vs. angle φ of wall slope of compressed CNTs (6,4)

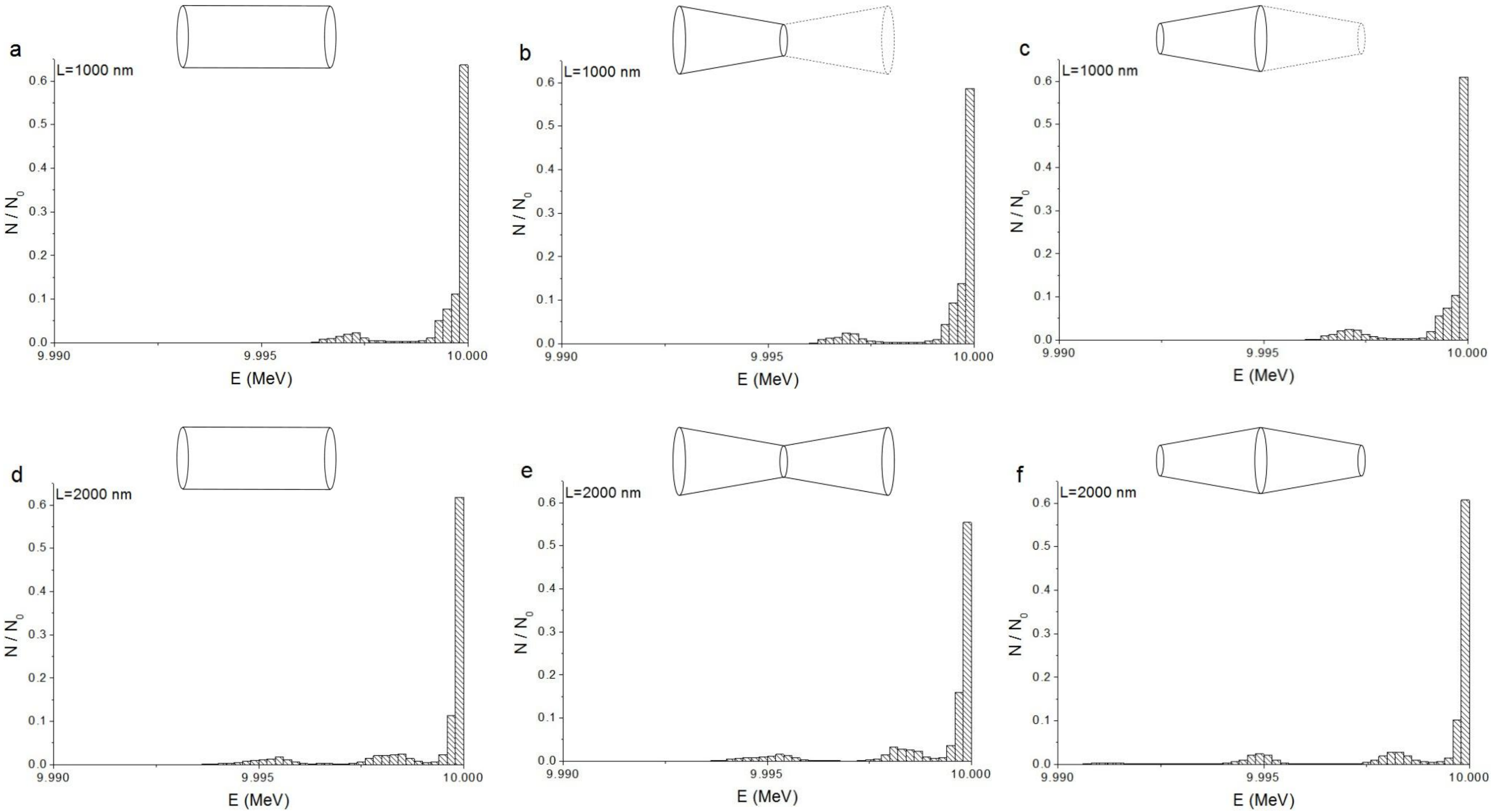
(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Comparison between straight and compressed CNTs (11,9) with φ = 0.005°

Energy distribution

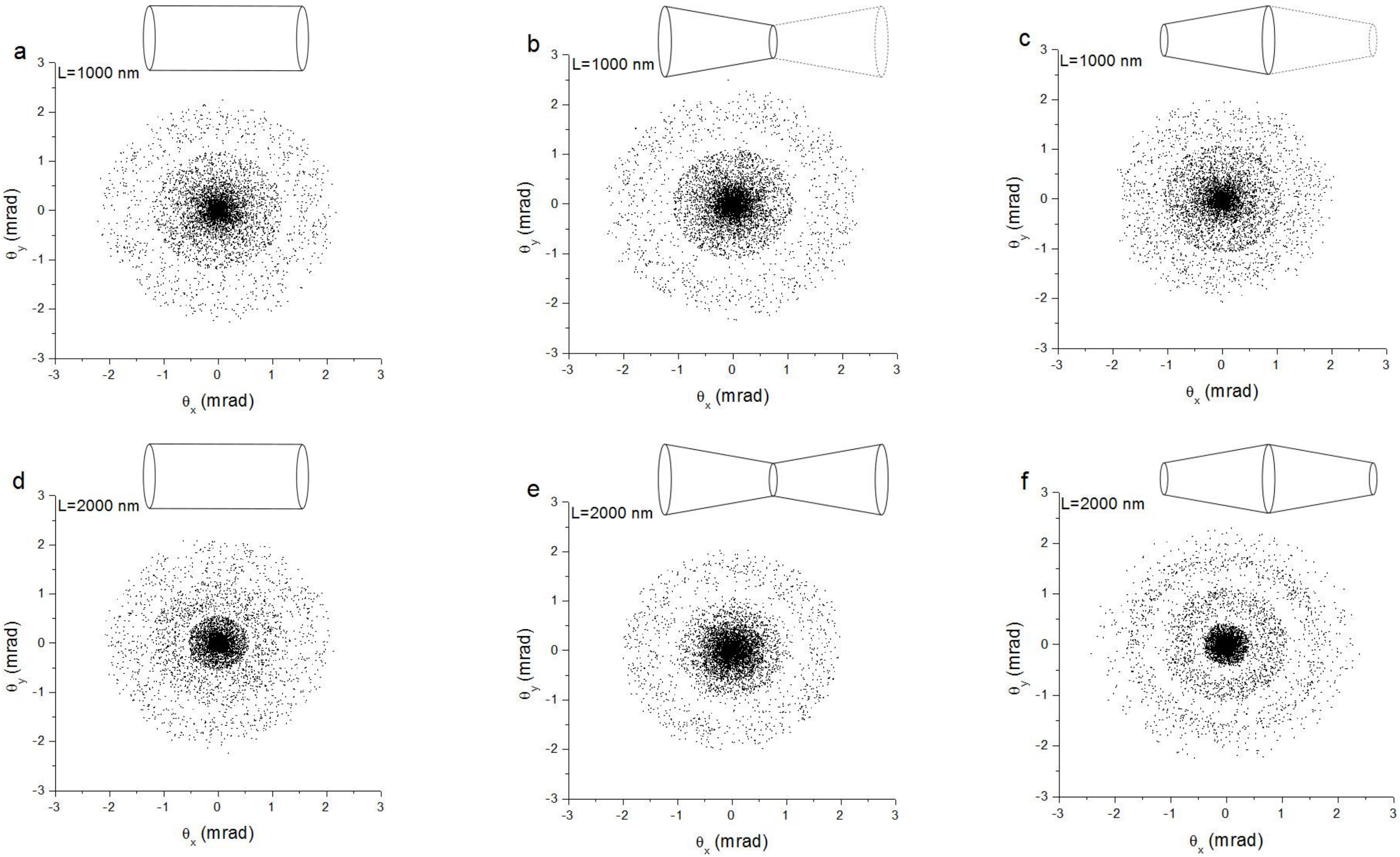
(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Comparison between straight and compressed CNTs (11,9) with $\varphi = 0.005°$

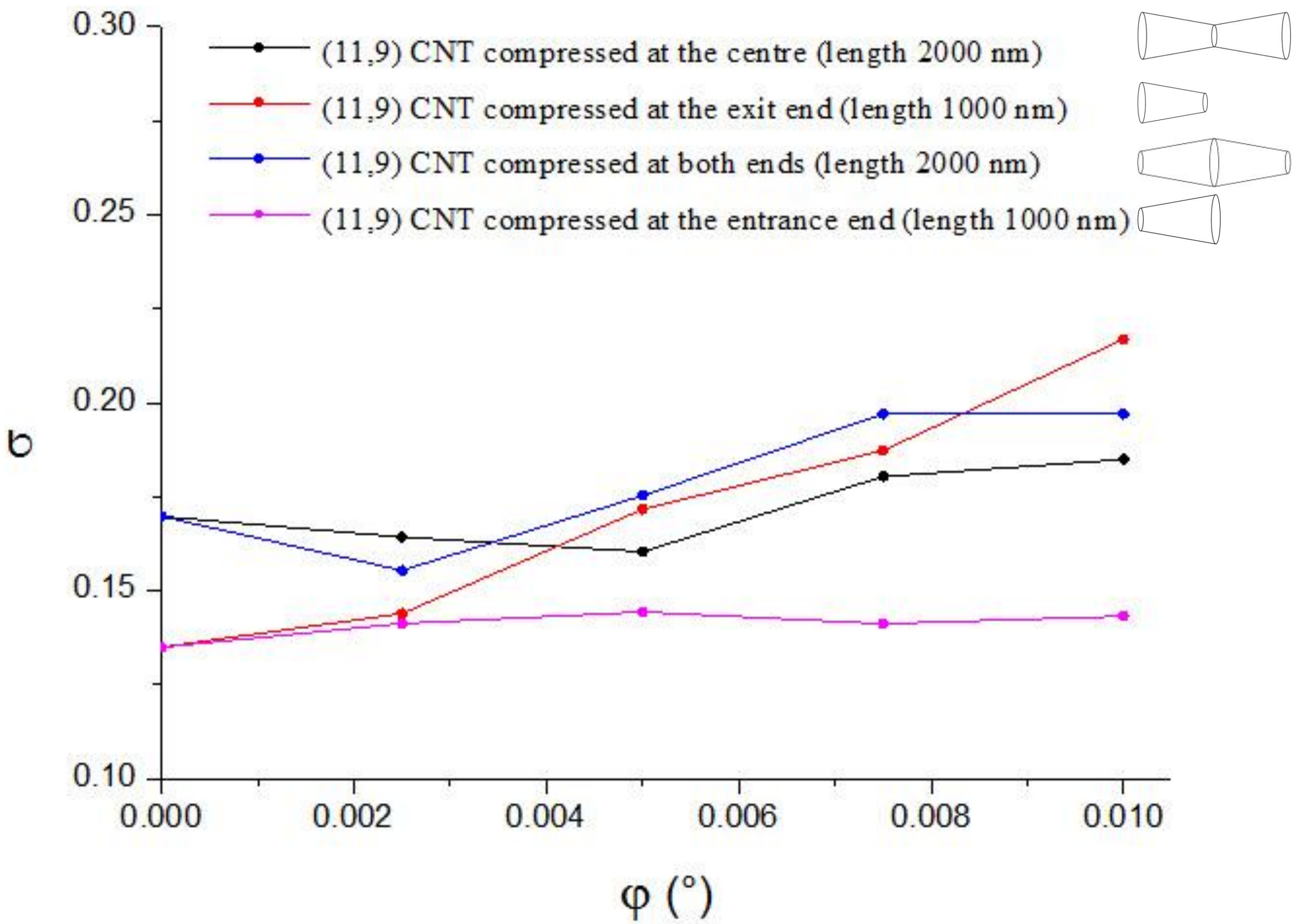
Angular distribution

(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Standard deviation vs. angle φ of wall slope of compressed CNTs (11,9)

(initial proton energy: 10 MeV, length of CNT: 1000 nm, 2000 nm)



Conclusions:

- In case of CNTs compressed at the centre proton beam exits **more collimated**, compared with straight CNTs or CNTs compressed at one end or at both ends, especially in **(6,4)** than in (11,9) CNT

- Energy distribution in case of (6,4) CNT compressed at the centre presents **high peaks**, compared with the main peak of maximum energy

Future tasks:

- Investigation of particle propagation in bundles of these compressed CNTs
- Consideration of different initial conditions (incident angle, beam collimation, energy spread)

Thank you for your attention!