Channeling-2024
11th September 2024

First-principles calculations of channeling of low-energy ions in SWCNTs and the effect of many-particle interactions

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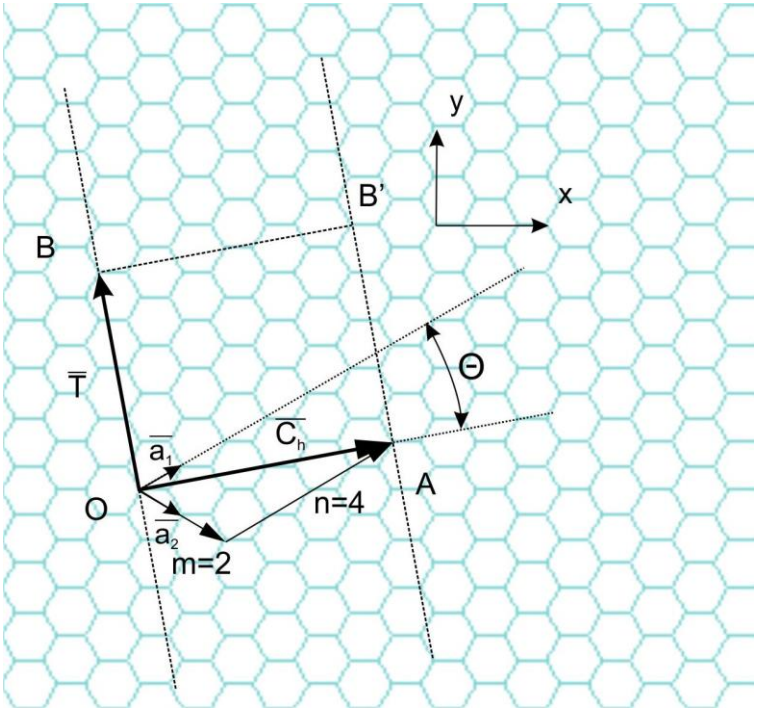
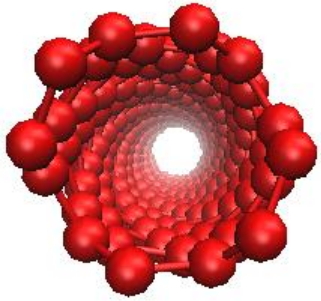
Presentation plan

- Review
- Methods
- Results
- Conclusions

Carbon nanotubes



Point **O** aligned with point **A**, and point **B** – with **B'**



УНТ(4,2)

$$\overrightarrow{C_h} = n\overrightarrow{a_1} + m\overrightarrow{a_2} \equiv (n,m); \qquad \overrightarrow{a_1} = \left(\frac{\sqrt{3}}{2}a, \frac{a}{2}\right); \quad \overrightarrow{a_2} = \left(\frac{\sqrt{3}}{2}a, -\frac{a}{2}\right);$$

$$\vec{T} = t_1\overrightarrow{a_1} + t_2\overrightarrow{a_2} \equiv (t_1,t_2), t_1, t_2 \in Z;$$

$$a = \sqrt{3} \times 0.144 \text{ нм}$$

$$t_1 = \frac{2m+n}{g_R}, t_2 = -\frac{2n+m}{g_R};$$

a – graphene lattice constant;

$$g_R = \begin{cases} g, \text{if } (n-m) \text{ isn't multiple of } 3g, \\ 3g, \text{if } (n-m) \text{is multiple of } 3g. \end{cases}$$

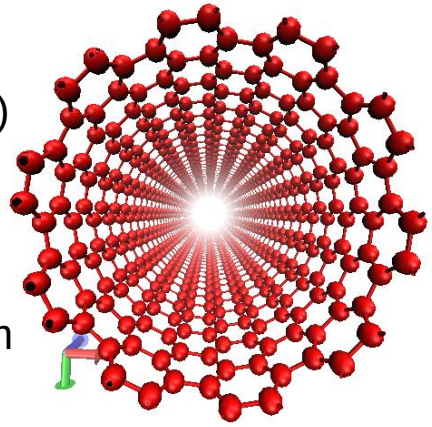
g – GCD(n,m);

$$\cos\theta = \frac{\overrightarrow{C_h} \cdot \overrightarrow{a_1}}{|\overrightarrow{C_h}| \cdot |\overrightarrow{a_1}|} = \frac{2n+m}{2\sqrt{n^2+m^2+nm}}.$$

θ – chirality

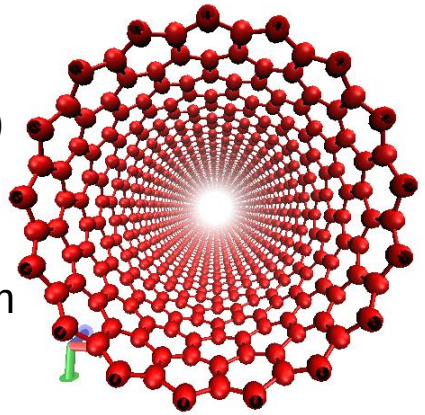
CNT(10,10)

D=1.36 nm



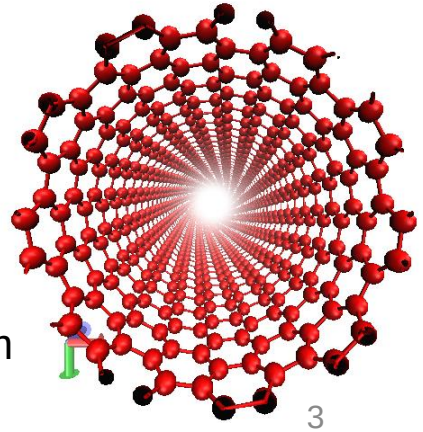
CNT(17,0)

D=1.33 nm



CNT(11,9)

D=1.36 nm

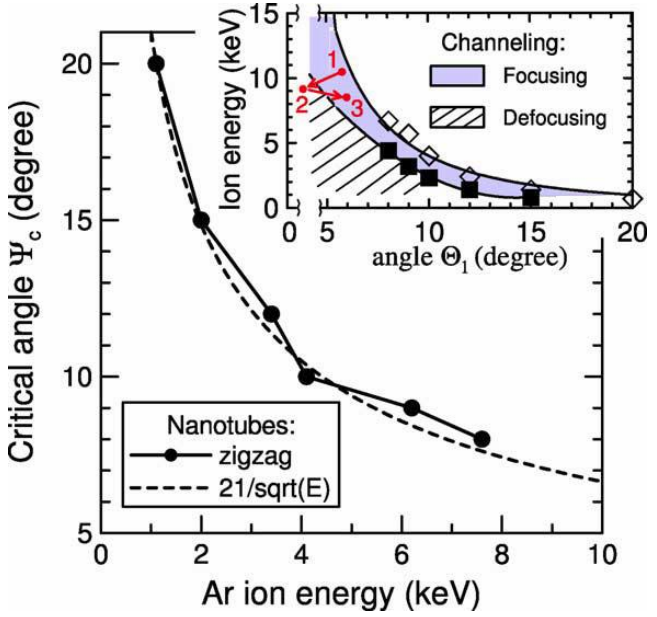


Studying the processes of ion movement through nanotubes taking into account the channeling effect

- Ion implantation using nanotubes is promising in a number of areas, such as medicine and chemistry.
- Carbon nanotubes can be used to **control ion beams** and also as **containers for storing matter**.
- During ion implantation, the beam is directed along the axis of the nanotube, while the ions move in the channeling mode, that is, they do not leave the tube and lose relatively little energy.

Features of channeling processes in nanotubes

- Carbon nanotubes are wider than crystalline channels.
- Due to the low density of electrons inside CNTs, the energy losses of ions during movement in nanotubes are small, therefore, the depths of penetration of channeled particles into CNTs significantly exceed the depths of penetration into single crystals.
- The critical channeling angles (maximum tube entry angles with respect to the axis at which ions move in the channeling mode) in CNTs are much larger than in crystals [1].

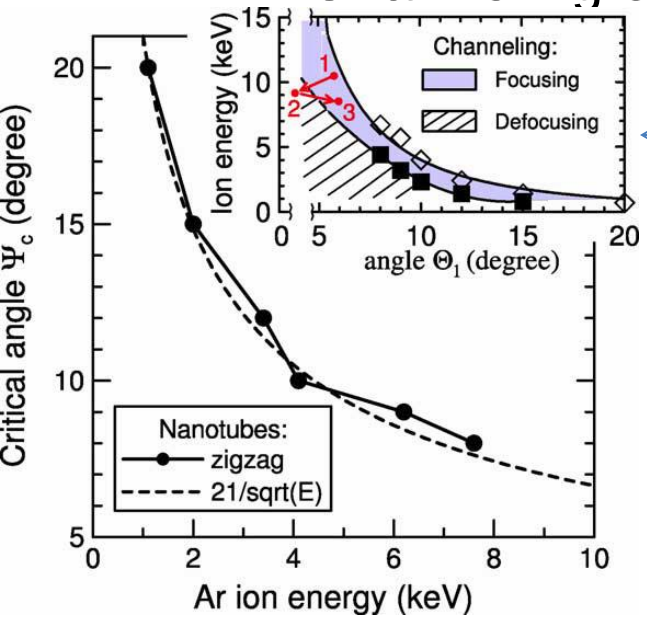


Channeling in CNTs is distinguished for three energy ranges:

- High ~GeV
- Average ~MeV
- Low ~keV

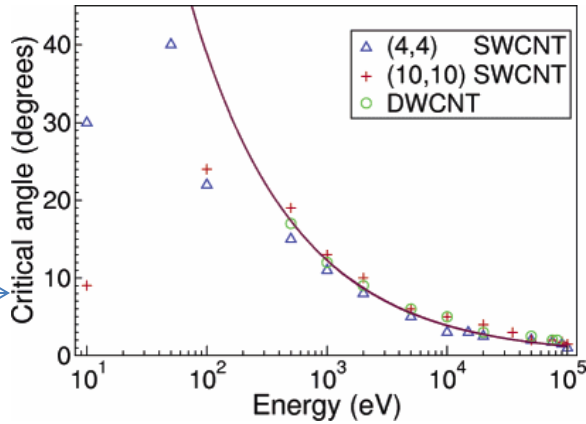
1. Mišković, Z.L., *Ion channeling through carbon nanotubes.* Radiation Effects and Defects in Solids, 2007. **162**(3-4): p. 185-205.
2. ***Zhiyuan Zhu et al. The experimental progress in studying of channeling of charged particles along nanostructure. Proc. SPIE 5974, 2006. P. 597413.***

Channeling of low-energy ions in carbon nanotubes



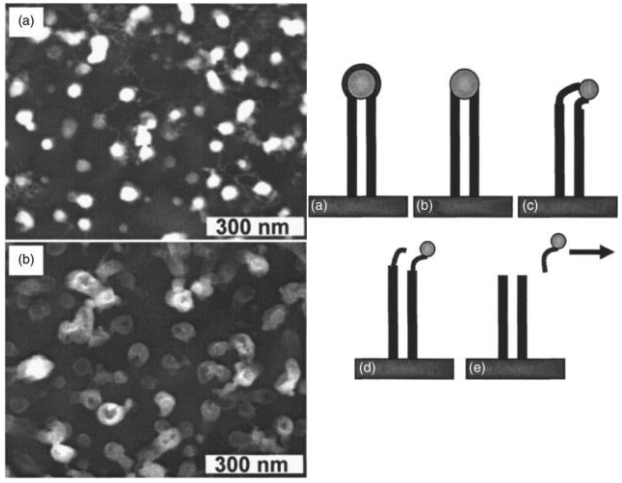
Critical angle as a function of ion energy for zig-zag nanotubes. [2].

Critical channeling angle of C+ ions in single-walled and double-walled carbon nanotubes as a function of energy. [3].

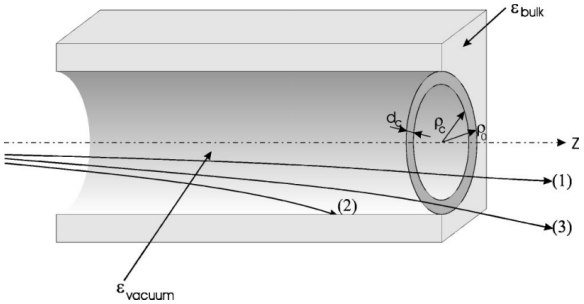


1. Dedkov, G.V., *Characterization of nanotubes as microscale beam manipulators: transmission of neutral atoms and low-energy ions. Surface and Coatings Technology, 2002.* ***158–159(0): p. 75-80.***
2. Krasheninnikov, A.V. and K. Nordlund, *Channeling of heavy ions through multi-walled carbon nanotubes. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2005.* ***228(1–4): p. 21-25.***
3. Moura, C.S. and L. Amaral, *Channeling on carbon nanotubes: a molecular dynamics approach. J Phys Chem B, 2005.* ***109(28): p. 13515-8.***
4. Wei, Z., et al., *Molecular dynamics study of a low energy carbon ion moving in a single-wall carbon nanotube. Nanotechnology, 2005.* ***16(11): p. 2681.***

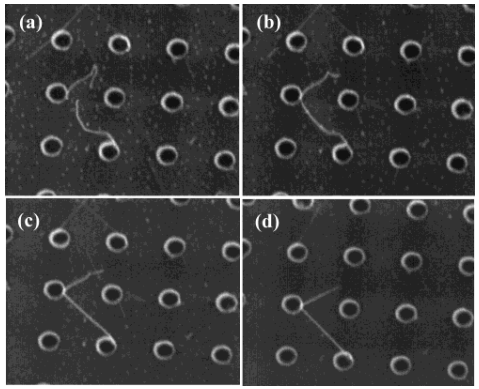
Opportunities for experimental verification of the channeling effect in nanotubes



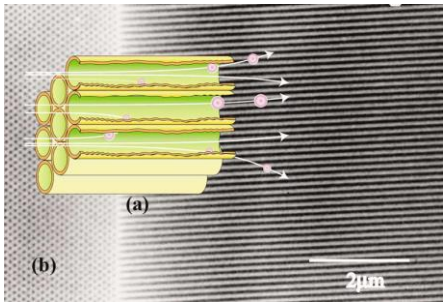
Opening the ends of CNTs using ion irradiation [1]



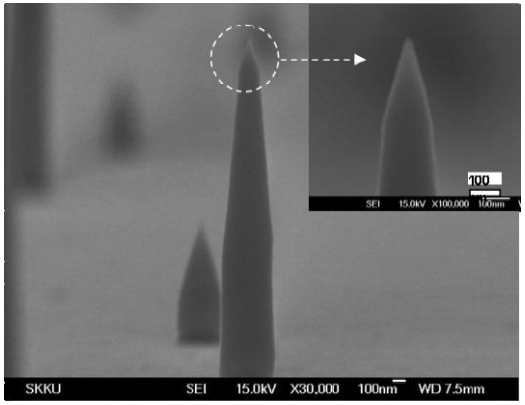
Channeling in the channels of holes in a thin metal foil [3]



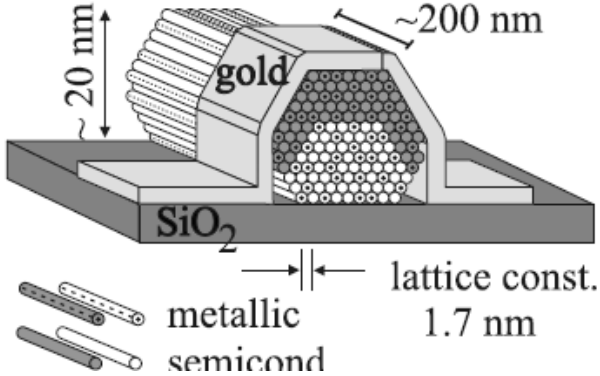
A network of CNTs hanging on nanocolumns SiO_2 [5]



Channeling in channels of holes in a thin porous alumina membrane [2]



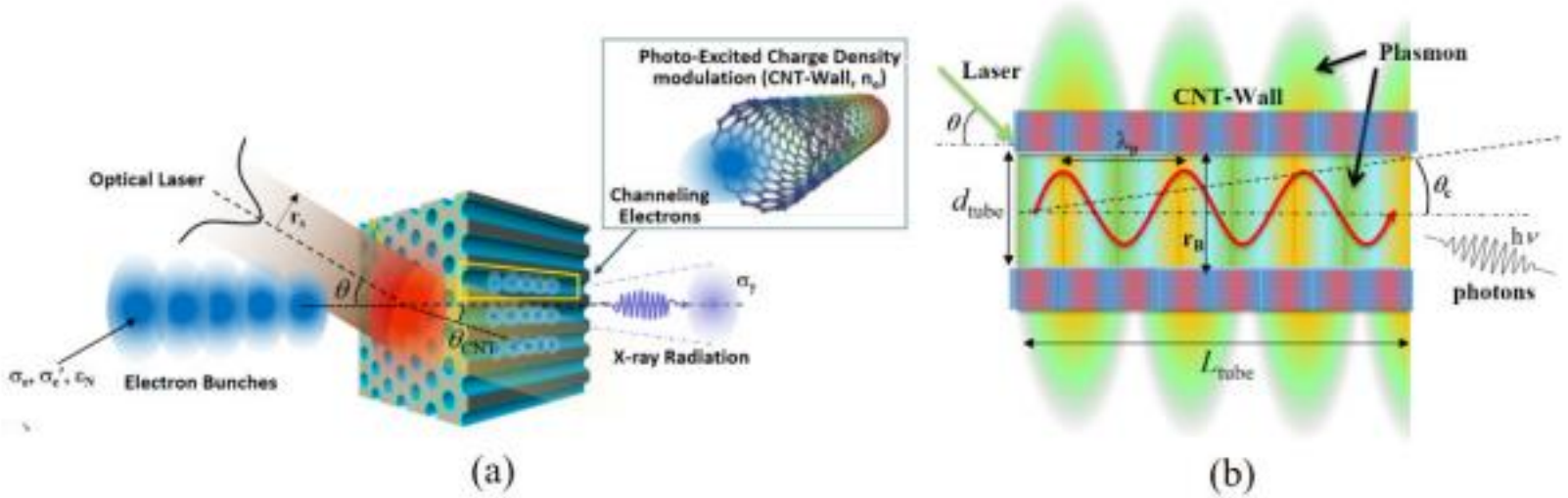
CNT growth in SiO2 track channels[4]



SWCNT bundle clamped with an Au bracket on a SiO2 substrate [6]

1. AuBuchon, J.F., et al., *Opening of aligned carbon nanotube ends via room-temperature sputter etching process.* Journal of Applied Physics, 2005. **97**(12)
2. Yamazaki, Y., *A microcapillary target as a metastable hollow ion source.* Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2002. **193**(1–4): p. 516-522.
3. Tőkési, K., et al., *Hollow-ion formation in microcapillaries.* Physical Review A, 2001. **64**(4): p. 042902.
4. Berdinsky, A.S., et al., *Growth of carbon nanotubes in etched ion tracks in silicon oxide on silicon.* Nano, 2007. **02**(01): p. 59-67.
5. Jung, Y.J., et al., *Straightening Suspended Single Walled Carbon Nanotubes by Ion Irradiation.* Nano Letters, 2004. **4**(6): p. 1109-1113.
6. Stahl, H., et al., *Intertube Coupling in Ropes of Single-Wall Carbon Nanotubes.* Physical Review Letters, 2000. **85**(24): p. 5186-5189.

Recent works of channeling phenomena in aligned-CNTs array



International Journal of Modern Physics AVol. 34, No. 34, 1943005 (2019)
https://doi.org/10.1142/S0217751X1943005X

The aim of the study

The aim of the work is to establish the effect of CNT wall perturbations caused by a particle moving along the channel on the motion of the particle

Limits of Applicability of the Classical Approach to Modeling the Processes of Particle Channeling in CNTs

I. $\lambda = \frac{h}{M_1 v} = \frac{h}{\sqrt{2 M_1 E_0}} \ll a_{C-C}$

λ – de Broglie wave length

M_1 – ion mass

v – ion velocity

h – Planck constant

E_0 – initial Energy of the particle

II. $4\pi \frac{l_{min}(\varepsilon)}{\lambda} \gg 1$

$l_{min}(\varepsilon)$ – closest approach

$$\varepsilon = \frac{M_2/M_1}{(1 + M_2/M_1)} \cdot \frac{E_0 a}{Z_1 Z_2 e^2}$$

M_2 – mass of a carbon atom

Z_1, Z_2 – nuclear charge of the ion and carbon atom

$a = 0.8854 a_B (Z_1^{0.23} + Z_2^{0.23})^{-1}$

III. $\delta(t) = \sqrt{\delta_0^2 + \frac{t^2}{4\,\delta_0^2\,M^2}}, \quad \delta \ll D,$

δ_0 – the initial width of the wave packet of the particle, D – CNT diameter,

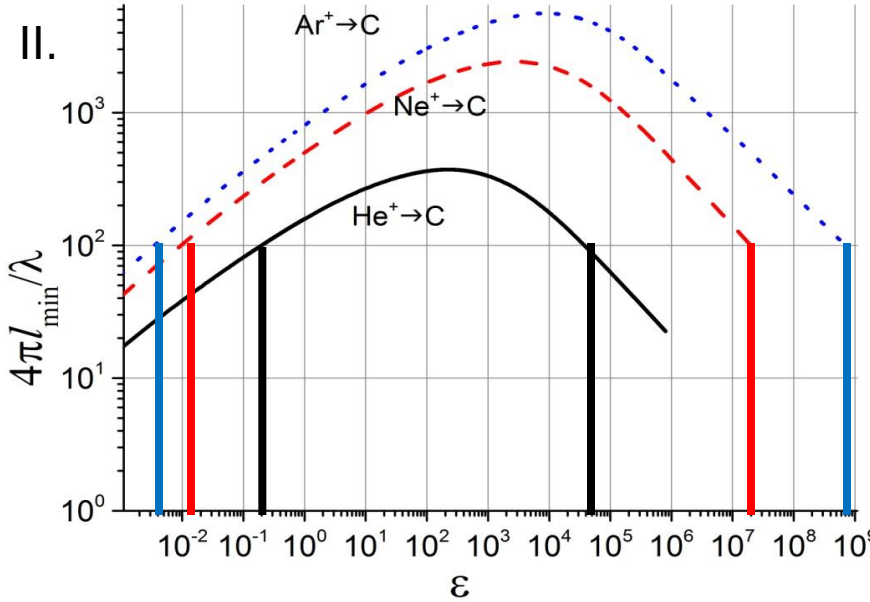
$t \cong 0.1$пс, t – time after $\delta = D$.

I. $\lambda = a_{C-C} = 0.142$ нм;

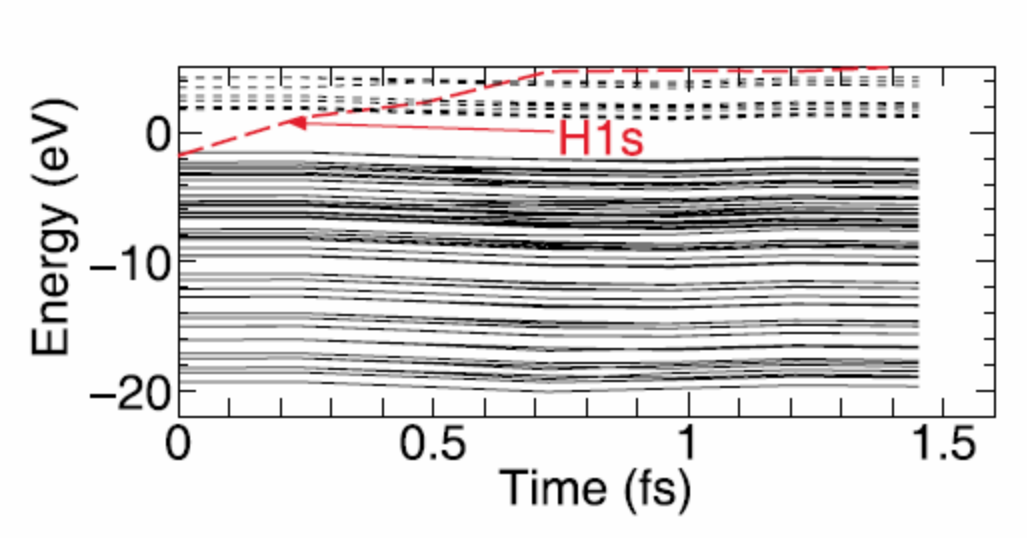
a_{C-C} is the interatomic distance in CNTs

Ion type	M, a.u.m.	Emin, eV
He	4.008	0.01
Ne	20.017	0.002
Ar	39.948	0.001

II.



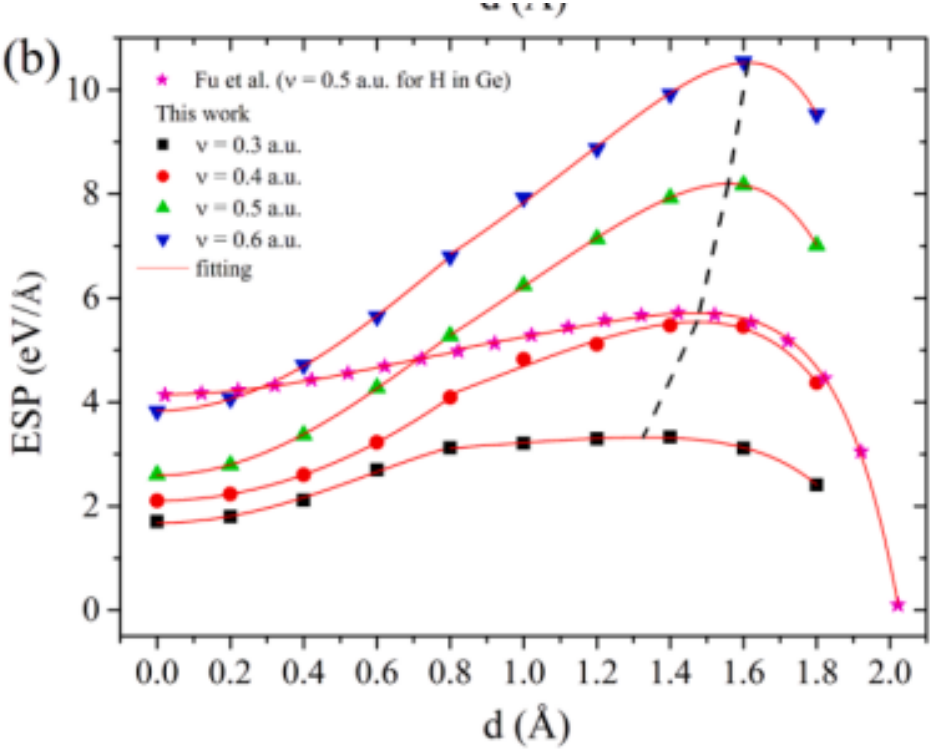
Ion neutralization



Time evolution of the Kohn-Sham energy at the moment of collision of the H atom with graphene. A hydrogen atom with an energy of 3 keV passed along the normal to the graphene plane to the center of the hexagon. After the collision, the hydrogen atom lost 20 eV [1].

1. Krasheninnikov A. V., Miyamoto Y., Tománek D. Role of Electronic Excitations in Ion Collisions with Carbon Nanostructures // Physical Review Letters. -- 2007. -- Vol. 99, No. 1. -- P. 016104.
2. G. Schiwietz et al., Nucl. Instrum. Methods Phys. Res., Sect. B 175–177, 1 (2001).

Energy transfer in single wall carbon nanotube



Zun-Yi Deng, Zhihua Hu, Hong-Jian Feng, Nonadiabatic energy transfer in single wall carbon nanotube upon H+ irradiation from time-dependent density-functional theory,
Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Volume 531, 2022, Pages 93-99, ISSN 0168-583X, https://doi.org/10.1016/j.nimb.2022.09.026.

Simulation method

Classical molecular dynamics equation system, LAMMPS code [1] (Large-scale **A**tomic/ **M**olecular **M**assively **P**arallel **S**imulator, 2009-2016)

$$m_i\ddot{\vec{r}}_i(t) = \vec{F}_i(\vec{r}), i = 1,2..N; \quad \vec{F}_i(\vec{r}) = -\frac{\partial U(\vec{r})}{\partial \vec{r}_i}, i = 1,2..N;$$

$$\vec{r} = \{\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n\}; \quad U(\vec{r})$$ – potential of interaction;

N - number of particles in the system

Solution of the equations of motion Werlet method in speed form:

$$\vec{v}_i\left(t + \frac{1}{2}\Delta t\right) = \vec{v}_i(t) + \Delta t\frac{\vec{F}_i(\vec{r}(t))}{2m_i}; \quad \vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{v}_i\left(t + \frac{1}{2}\Delta t\right)\Delta t;$$

$$\vec{v}_i(t + \Delta t) = \vec{v}_i\left(t + \frac{1}{2}\Delta t\right) + \frac{\Delta t}{2m_i}\vec{F}_i(\vec{r}(t + \Delta t)).$$

Periodic Born-Karman Boundary Conditions

$$\begin{cases} x_{min} \le x_i \le x_{max}, \\ y_{min} \le y_i \le y_{max}, \\ z_{min} \le z_i \le z_{max}. \end{cases} \qquad \begin{matrix} a, b, c_{min,max} \\ x, y, z_{min,max} \end{matrix}$$ – simulation box borders

$$x_i^j = x_i - (a_{max} - a_{min}) + a_{min}, j_i = j_i + 1$$

Non-periodic boundary conditions

$$\begin{cases} a_{min} \le x_i \le a_{max}, \\ b_{min} \le y_i \le b_{max}, \\ c_{min} \le z_i \le c_{max}. \end{cases}$$

Potential of interaction of carbon atoms AIREBO [2]:

$$E_{AIREBO} = \sum_i \sum_{j(>i)} [V^R(r_{ij}) - b_{ij}V^A(r_{ij}) + V^{LJ}(r_{ij})]$$

Repulsive part:

$$V^R(r_{ij}) = f^c(r_{ij}) \cdot (1 + Q/r_{ij}) \cdot Ae^{-\alpha r_{ij}}$$

Attractive part:

$$V^A(r_{ij}) = f^c(r_{ij}) \cdot \sum_{n=1,3} B_n e^{-\beta_n r_{ij}}$$

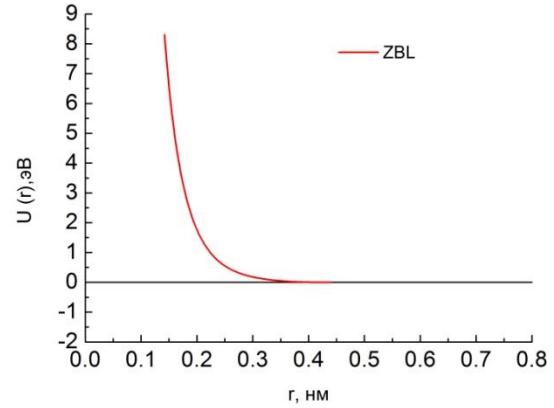
$$f^c(r_{ij}) = \begin{cases} 1, r \le D_{ij}^{min} \\ \left[1 + \cos\left(\frac{(r - D_{ij}^{min})}{(D_{ij}^{max} - D_{ij}^{min})}\right)\right]/2, D_{ij}^{min} < r \le D_{ij}^{max} \\ 0, r > D_{ij}^{max} \end{cases}.$$

D_{min}=0.18nm; D_{max}=0.2 nm

1. Plimpton, S., *Fast Parallel Algorithms for Short-Range Molecular Dynamics.* Journal of Computational Physics, 1995. **117**(1): p. 1-19
2. Stuart, S.J., A.B. Tutein, and J.A. Harrison, *A reactive potential for hydrocarbons with intermolecular interactions.* The Journal of Chemical Physics, 2000. **112**(14): p. 6472-6486

Interaction of an incident particle with a carbon atom

Interaction potential incident particle – carbon atom [1]:



$$V_{ZBL}(r) = f^c(r_{ij})\frac{Z_1 Z_2}{r}\sum_{i=1}^{4} a_i e^{-b_i \cdot \frac{r}{a}},$$

Z_1, Z_2 – the ion and the carbon atom nucleus charges;

$$a = 0.8854 a_B (Z_1^{0.23} + Z_2^{0.23})^{-1}$$ – shielding constant;

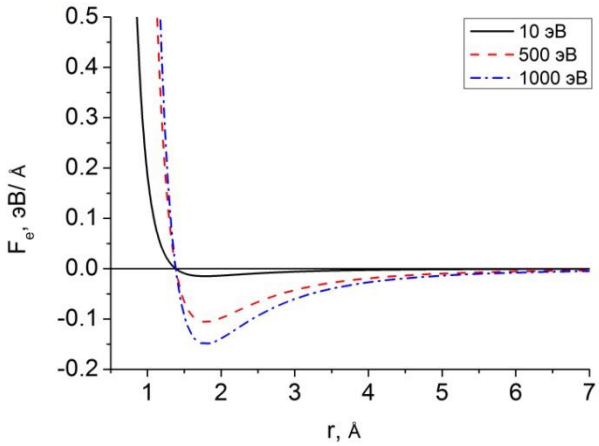
$$a_i = [0.1818, 0.5099, 0.2802, 0.02817]$$

$$b_i = [3.2, 0.9423, 0.4029, 0.2016]$$ – expansion coefficients[1];

$$f^c(r_{ij}) = \begin{cases} 1, r \le D_{ij}^{min} \\ \left[1 + \cos\left(\frac{(r - D_{ij}^{min})}{(D_{ij}^{max} - D_{ij}^{min})}\right)\right]/2, D_{ij}^{min} < r \le D_{ij}^{max} \\ 0, r > D_{ij}^{max} \end{cases}$$ – cutoff function;

D_{min}=0.4 nm; D_{max}=0.44 nm

Electron stopping power [2, 3]:



$$F_e = -\frac{q_1^2 \gamma v}{8\omega_s^2 \rho^3} - 3\frac{q_1^2 v}{2\pi}\frac{\ln(0.692 k_F \rho)}{(k_{TF}\rho)^4}$$

$k_F = v_F = \pi k_{TF}^2/4$, k_F - wave number,

q_1 – ion charge, ρ - distance to the CNT wall,

ω_s – surface plasmon frequency [3],

γ – friction coefficient [3], v – ion speed,

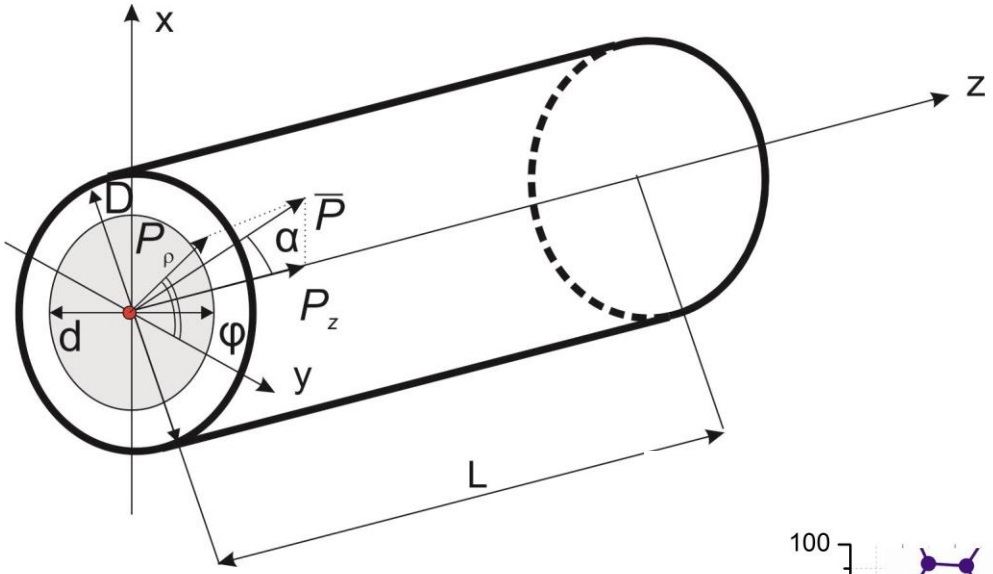
Hartree system of units (e=1, m_e=1, h=1)

1. Ziegler, J. and J. Biersack, *The Stopping and Range of Ions in Matter*, in *Treatise on Heavy-Ion Science*, D.A. Bromley, Editor. 1985, Springer US. p. 93-129.
2. Nunez, R., P.M. Echenique, and R.H. Ritchie. // Journal of Physics C: Solid State Physics, 1980. Vol. **13**(22): P. 4229.
3. Dedkov G. V. // Surface and Coatings Technology. -- 2002. – Vol. 9 -- 158–159, -- P. 75-80.
4. *Sadovnichy V., Tikhonravov A., Voevodin Vl., et al.* // Contemporary High Performance Computing: From Petascale toward Exascale. Boca Raton: CRC Press, 2013. P. 283.

TD-DFT Calculation details

- TD-DFT Octopus code
- Ehrenfest MD
- E cuttof =400 Ry
- SWCNTs(5,0) to (10,10) with 1*1*12 unit cell

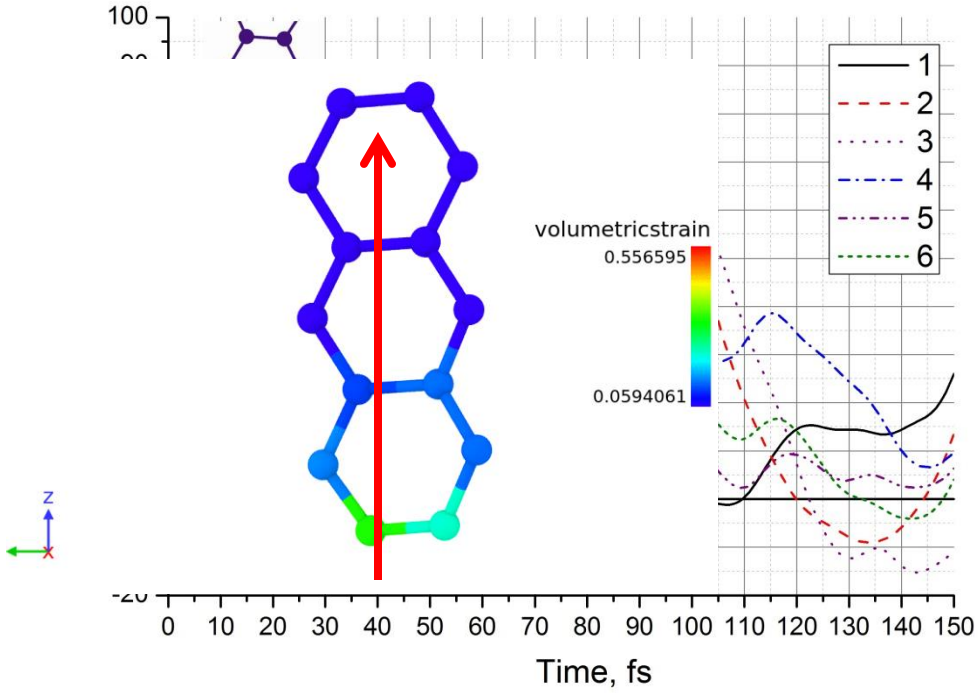
Molecular dynamic simulation initial condition



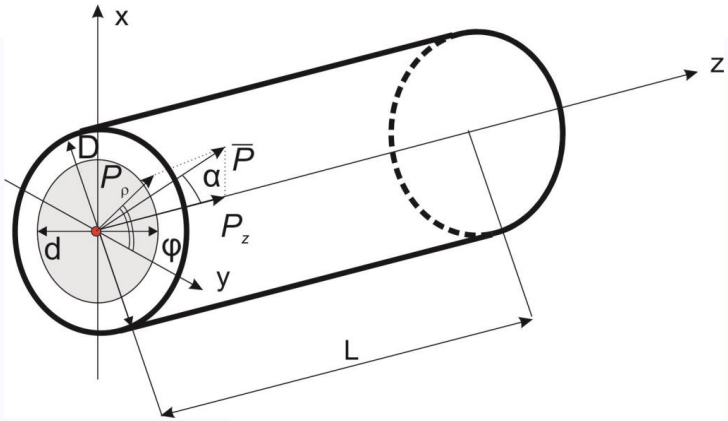
α – incident angle
φ – azimuthal angle
P – incident energy of the ion
D – CNT diameter
d - cross-sectional diameter of ion entry into CNT

Calculation parameters

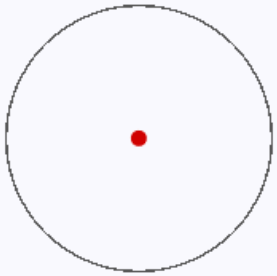
CNT (11,9), (10,10), (17,0)
T=300K,
D=1.36 nm,
Ar^+
α =20°,
φ =0°,
E_0 =100 eV.

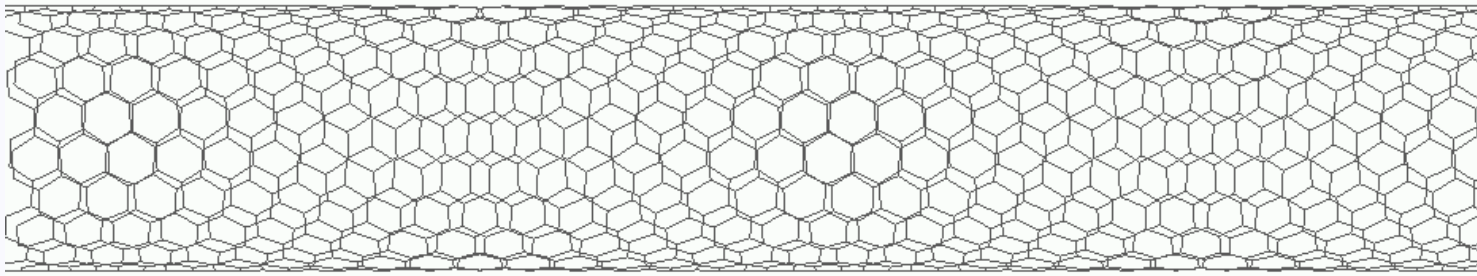


Many-Particle Effects in the Channeling of Atomic Particles



α – incident angle
φ – azimuthal angle
P – incident energy of the ion
D – CNT diameter
d - cross-sectional diameter of ion entry into CNT
L – nanotube length





C. S. Moura, L. Amaral // J Phys Chem B. – 2005. – V. 109, № 28. – P. 13515-8.

CNT parameters

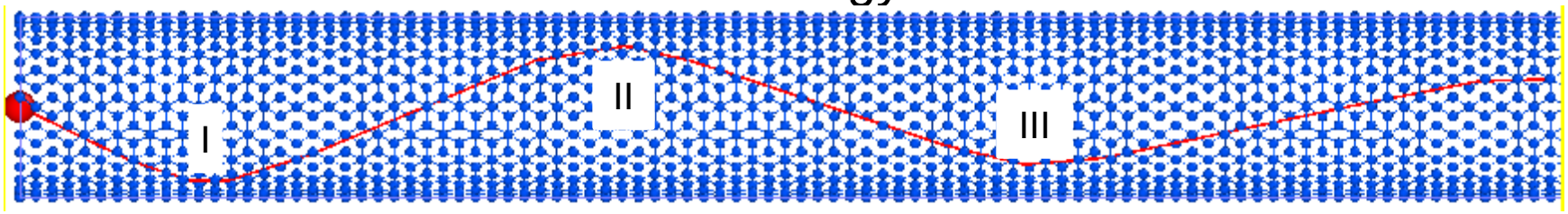
CNT type	D, nm
(10,10)	1.36
(17,0)	1.33
(11,9)	1.36

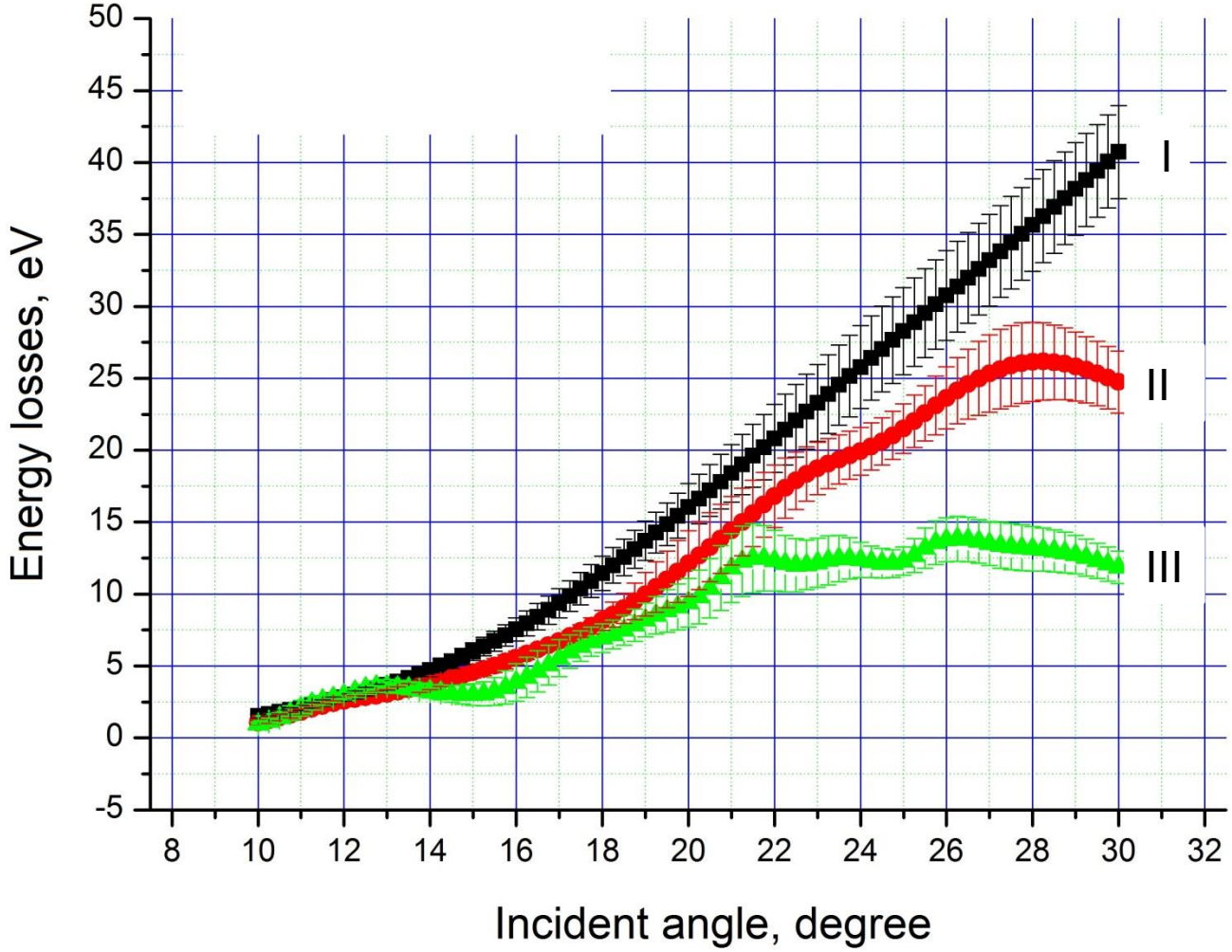
T=300K и 0.1K

Ion parameters

Z_0, nm	α_0, degree.	φ_0, degree	(x_0, y_0) nm	Ion type	E, eV	Number of incidents
0 - 0.24	10-30	-18—+18	(0,0)	Ar^+	100	13689

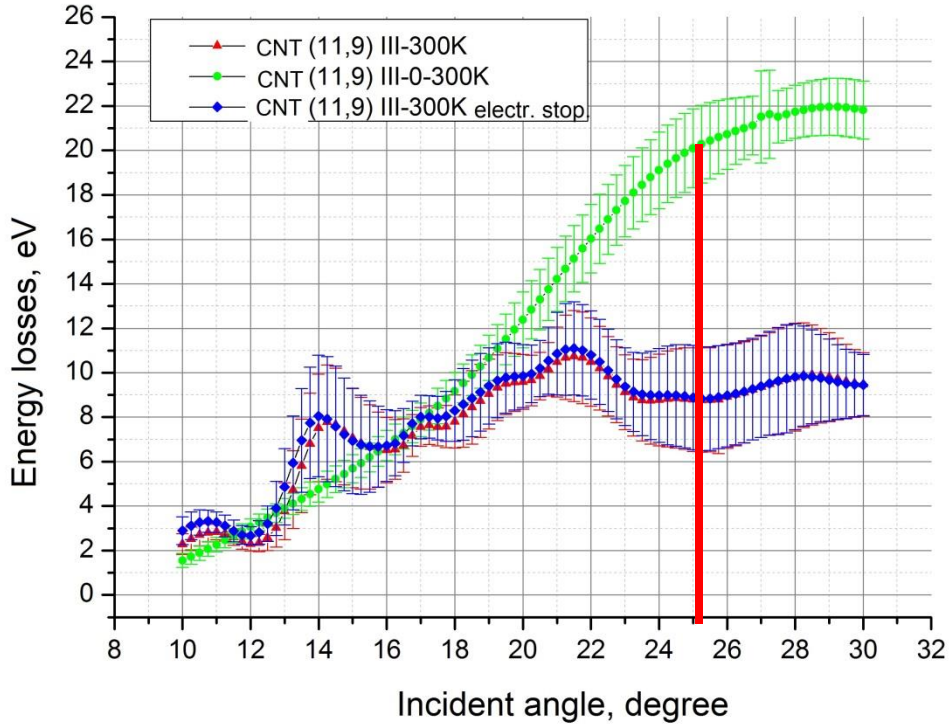
Ar^+ Ion Energy Loss

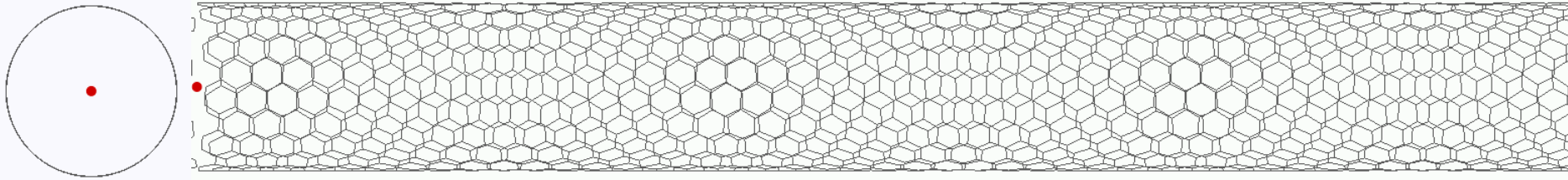




CNT(11,9)
E_0=100 eV

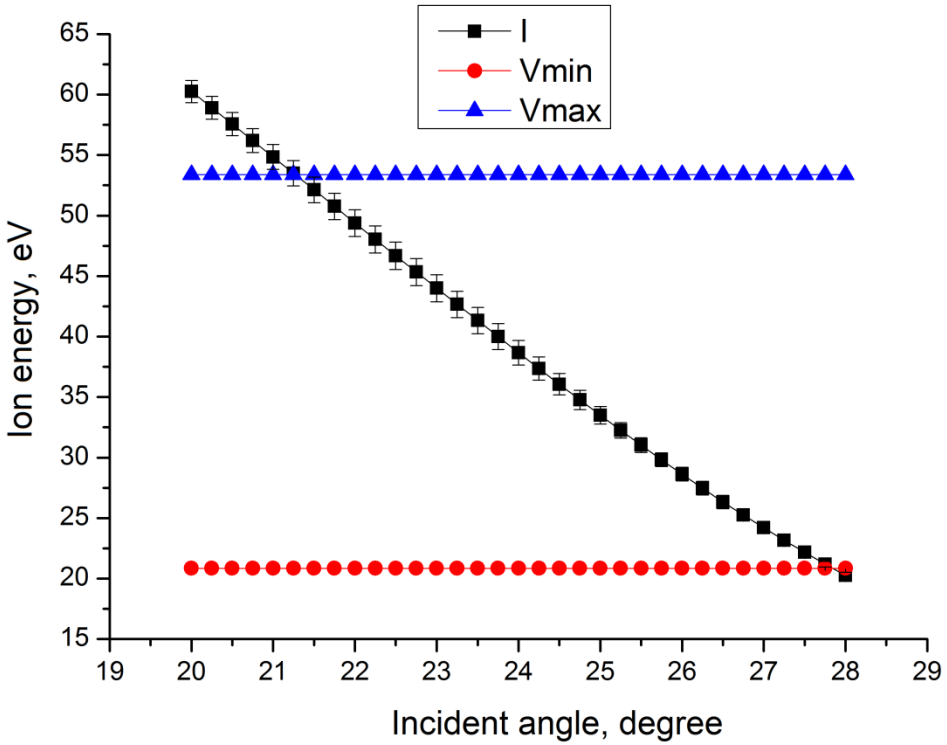
Energy loss by a particle with and without allowance for wall perturbation during motion Ar^+ (E_0=100 эВ) in SWCNT(11,9) at the third collision with the wall.





Ar^+ ion trajectory (E_0=100 eV) in CNT (11,9) with incident angle 25°

Determination of the particle energy range in which the interaction with the perturbation takes place



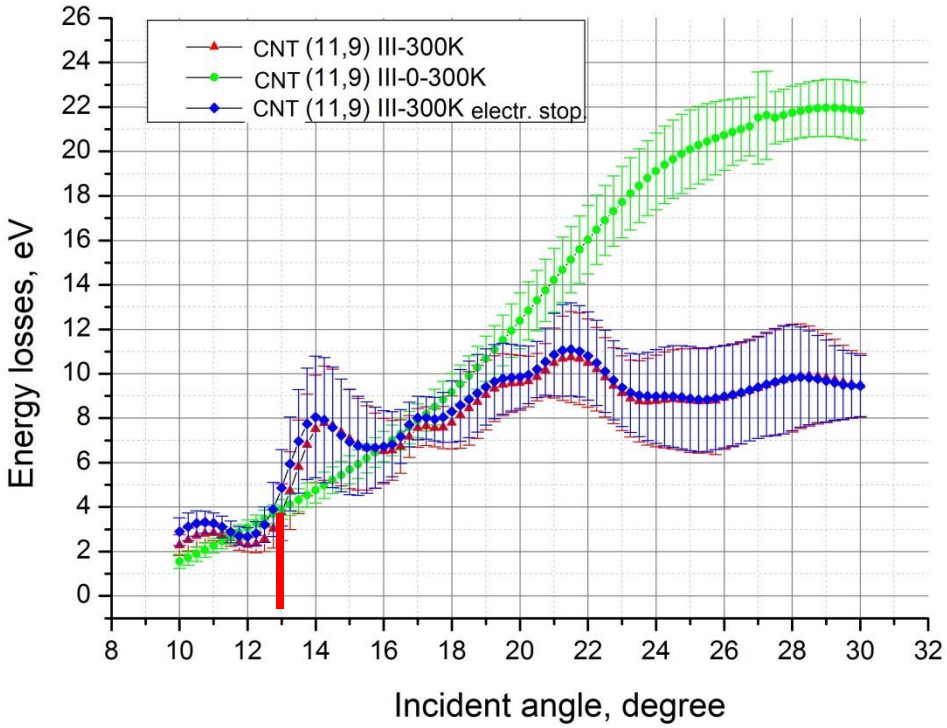
Phonon type	Velocity, km/s	Velocity, Å/ps
TA	9.1	91
LA	21.0	210
TW	16.2	162

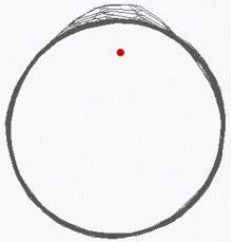
Disturbance movement speed ~150 Å/ps =15 km/s;

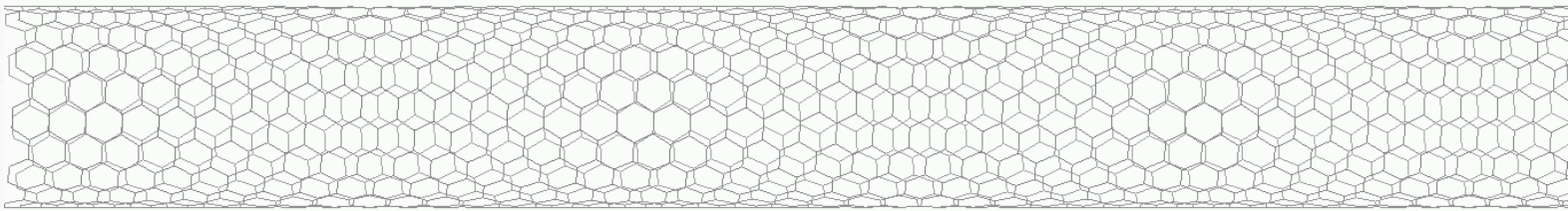
Longitudinal particle velocity 100 – 160 Å/ps = 10 – 16 km/s

I –the energy of the particle after the first collision with the wall.
Emin, Emax – lower and upper limits of the kinetic energy of ion motion Ar^+ with an initial energy of 100 eV flies into the tube (11.9) at different angles, at which the ion velocity is close to the perturbation propagation velocity; in this case, an interaction of the ion and the perturbation arises.

Energy losses during the third collision depending on the angle of entry with and without allowance for the perturbation

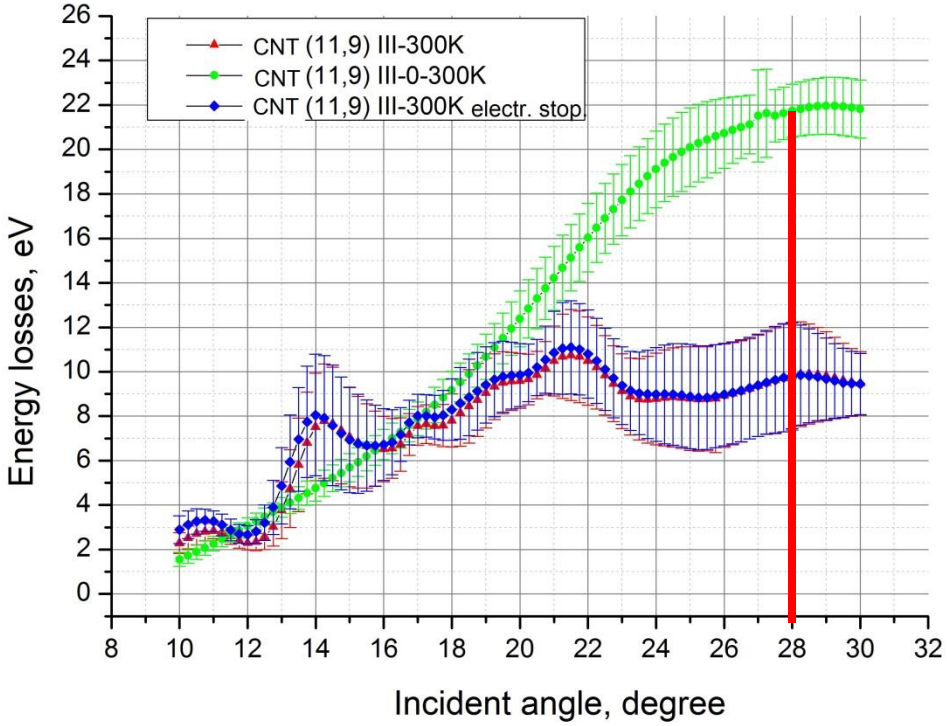


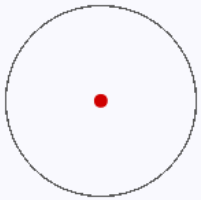


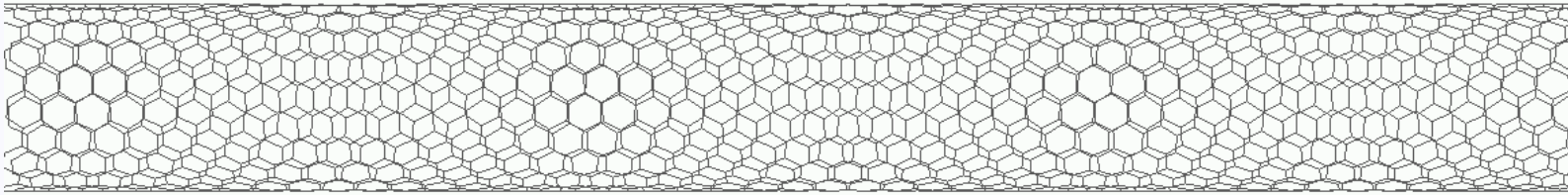


Trajectory of Ar^+ (E0=100) in CNTs (11.9) at an angle of entry of 13°

Energy loss during the third collision depending on the angle of entry, taking into account the perturbation

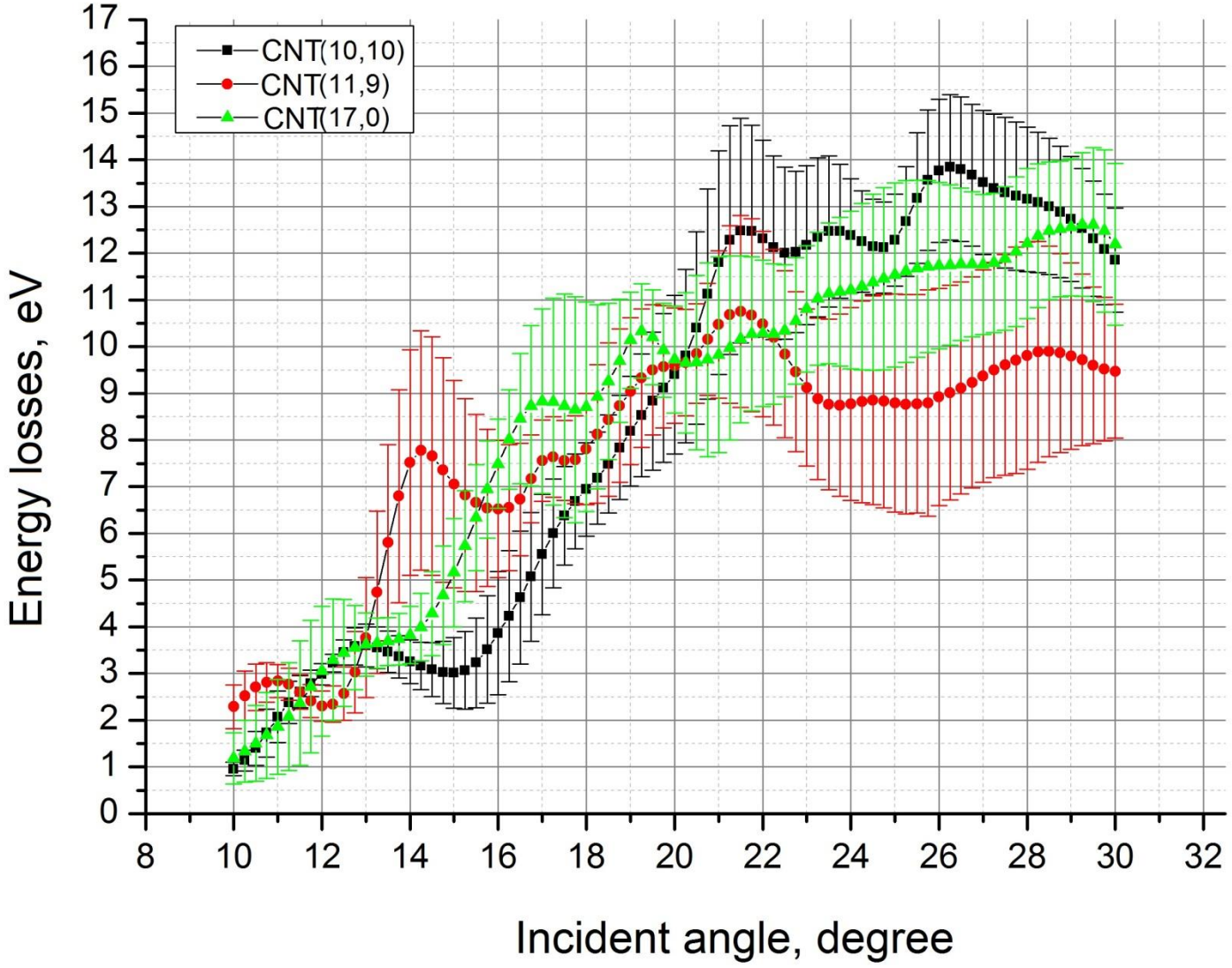




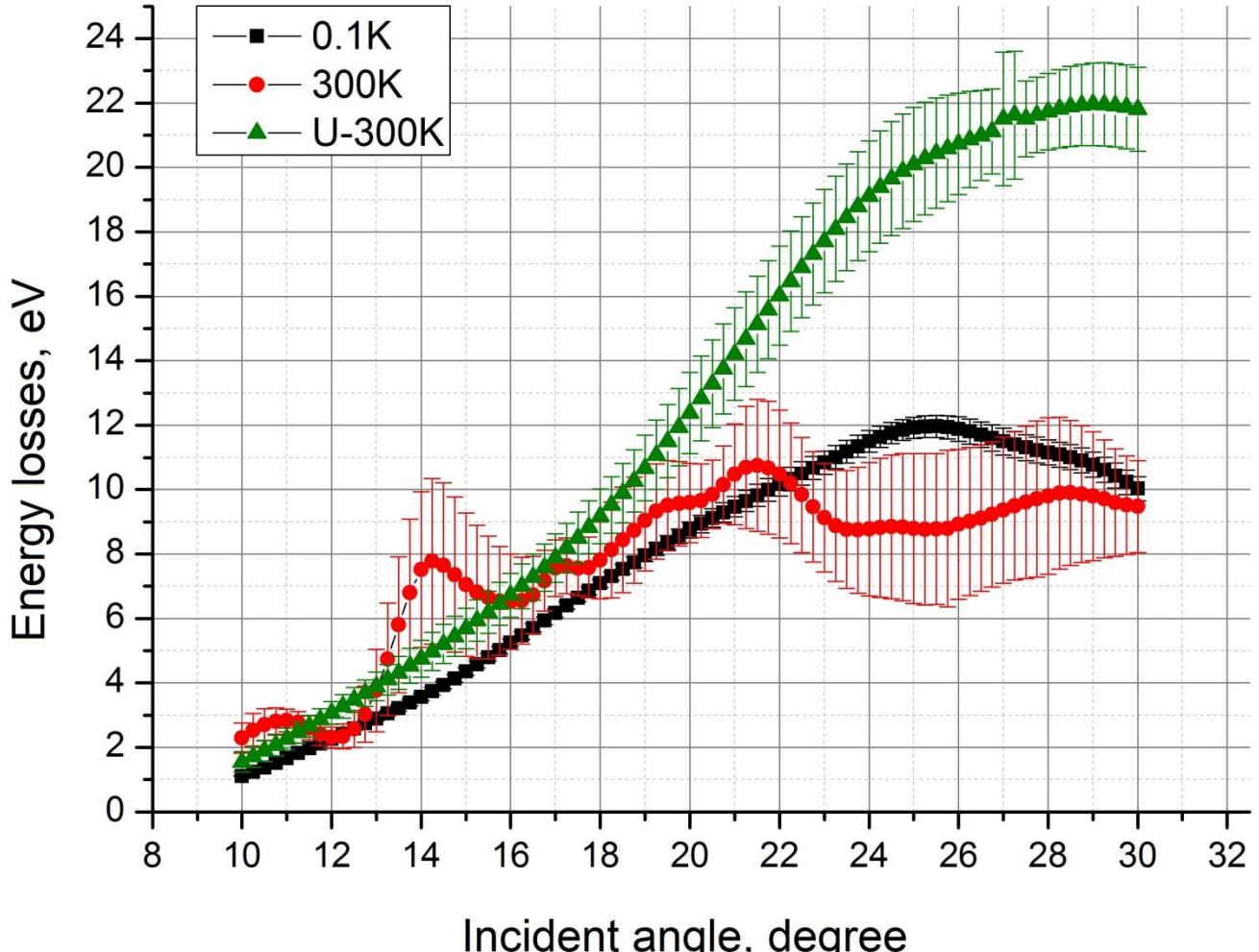


Trajectory of Ar^+ (E0=100) in CNTs (11.9) at an angle of entry of 28°

Energy loss during the third collision of the Ar+ ion with the CNT wall for "chair" (10.10), "chiral" (11.9) and "zig-zag" (17.0) nanotubes



Energy loss for Ar+ in the third collision with the CNT wall (11.9) with allowance for the perturbation of the CNT wall at different initial temperatures CNT 300 K and CNT 0.1 K with allowance for the perturbation and without perturbation of the CNT wall at 300 K



Conclusions

1. Channeled in carbon nanotubes (CNTs), low-energy particles with masses of 4–40 a.m.u., interacting with the elastic perturbations of the nanotube wall caused by them, lose less energy than with the same motion parameters without taking into account the perturbation, if the particle velocities are close to to the propagation velocity of the perturbation.
2. Taking into account the perturbation during the channeling of particles with angles close to critical, for a CNT temperature of 300 K, in contrast to 0.1 K, the dependence of energy losses during collisions with the wall is fluctuating. If perturbations are not taken into account, fluctuations are practically absent at both temperatures.

Thank you for your attention!