

Fast ion passing through straight and bent nanotubes

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Abstract

The motion of fast positively charged particles in straight and bent nanotubes and ropes of nanotubes is considered. The possibility of the dynamical chaos phenomenon at scattering of such particles by nanotube is shown. The deflection of fast ions by a bent rope of nanotubes is demonstrated.

Keywords: High-energy particle; Nanotube; Nanotubes rope; Channeling; Beam deflection

1. Introduction

A single wall nanotube is a hollow cylinder, whose surface consists of periodically located carbon atoms [1–3]. The transversal size of a nanotube can make tens of angstrom and the longitudinal size can reach hundreds of micron. The nanotube atoms form a deep and wide channel, along which the channeling of positively charged particles is possible. Attention was paid on this circumstance in [4,5]. In those works the particle motion in a field of nanotube was considered under the condition that the nanotube potential has cylindrical symmetry. In [6,7] it was shown that taking into account the azimuthal inhomogeneity of the nanotube potential makes

possible for an essential change of a particle motion characteristics. Specially, in [7] it was shown the possibility of a dynamical chaos phenomenon during channeling of positively charged particles in the field of a nanotube.

The composition of nanotubes can form a periodical structures – the nanotube ropes [1,8,9]. For such structures the nanotubes axes are parallel one to another and are situated periodically in the orthogonal plane. This paper is devoted to the investigation of a fast positively charged particle motion in such structures. The main attention is paid on the particle scattering in straight and bent nanotube ropes. We give some results of a simulation for passing of fast ions through straight and bent nanotubes rope, which was obtained by taking into account the azimuthal inhomogeneity of the nanotube potential. We will show that it is possible to observe a dynamical chaos phenomenon during the scattering of the particles by a nanotube. The possibility of a fast ion deflection by a bent rope of nanotubes will be shown.

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2. The motion of fast positively charged particles in the field of nanotubes rope

The motion of a fast charged particle in the field of nanotubes at small angle ψ relative its axis (z -axis) is determined mainly by a continuous potential of the nanotube, i.e. by the potential of the nanotube, averaged over the z coordinate

$$U_n(\boldsymbol{\rho}) = \frac{1}{L} \int_{-\infty}^{+\infty} dz \sum_i u(\mathbf{r} - \mathbf{r}_i), \quad (2.1)$$

where $u(\mathbf{r} - \mathbf{r}_i)$ is the potential of the nanotube atom located in the point \mathbf{r}_i , $\boldsymbol{\rho} = (x, y)$ are the coordinates in the plane, orthogonal to the nanotube axis and L is the nanotube length.

Nanotubes are formed in the rope of a periodic hexagonal structure in the orthogonal plane with the distance between neighboring nanotubes equals to 0.315 nm [9,10]. The total potential of such structure is equal to the sum of nanotubes potentials

$$U(\boldsymbol{\rho}) = \sum_k U_n(\boldsymbol{\rho} - \boldsymbol{\rho}_k), \quad (2.2)$$

where $\boldsymbol{\rho}_k$ is the position of nanotubes axis in the orthogonal plane. An example of such potential is presented on Fig. 1(a). The Molire approximation [11] for the potential of a single atom was used for calculation.

The momentum component p_{\parallel} parallel to the z -axis is conserved in the field (2.2). In this case the motion in the transversal plane will be determined by the two-dimensional equation

$$\ddot{\boldsymbol{\rho}} = -\frac{1}{\varepsilon_{\parallel}} \frac{\partial}{\partial \boldsymbol{\rho}} \mathbf{U}(\boldsymbol{\rho}), \quad (2.3)$$

where $\varepsilon_{\parallel} = \sqrt{p_{\parallel}^2 + m^2}$ and m is the particle mass (the velocity of light c equals unity). For high-energy particles moving along the nanotube axis the value ε_{\parallel} is close to the energy ε of incident particle. Therefore, below, we suppose that $\varepsilon_{\parallel} \approx \varepsilon$.

As is well known [4–7], the integral of the energy of transversal motion is conserved in the field (2.3)

$$\varepsilon_{\perp} = \frac{\varepsilon \dot{\boldsymbol{\rho}}^2}{2} + \mathbf{U}(\boldsymbol{\rho}). \quad (2.4)$$

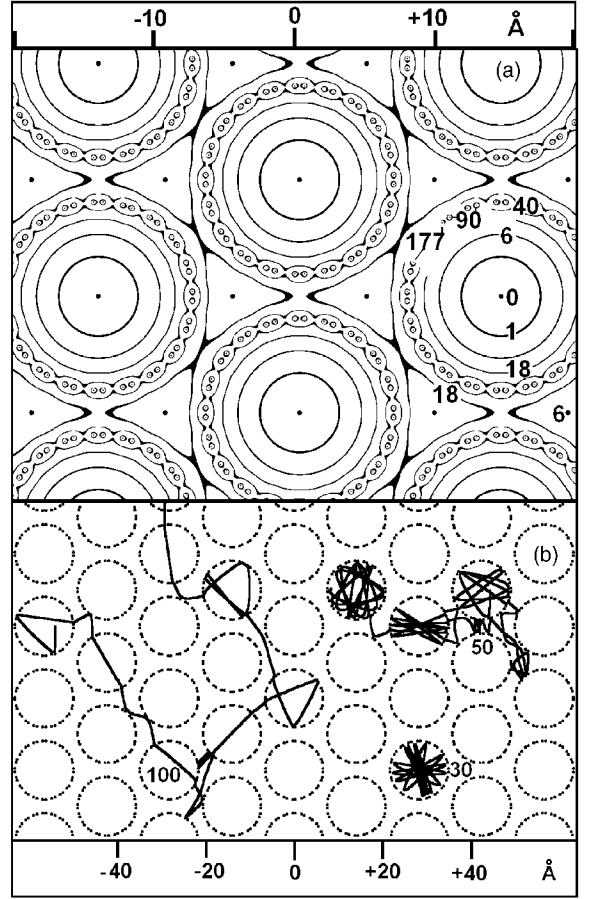


Fig. 1. Equipotential surfaces for proton interaction with a continuous potential field of a nanotube (10, 10) rope in the plane orthogonal to its axis (a), and typical trajectories of positively charged particles in such field (b). Numbers near the curves correspond to the potential levels values in eV (a), and to the transverse energy of the particles in eV (b).

In dependence from the value ε_{\perp} the particle motion can be finite (channeling) or infinite in the transversal plane of the nanotubes rope.

Thus, the problem of a fast particle motion in the nanotubes rope is similar to the problem of a particle motion in the periodic field of crystal atomic strings (see [12,13] and references herein). The only difference is that the continuous potential of crystal atomic strings has maxima on the axis of each string, while in the nanotubes rope the potential maxima are on the surface of each nanotube. The potential minima of each nanotube are on its centerline (axis) (see Fig. 1(a)).

On Fig. 1(b) the typical trajectories of positively charge particle in the transversal plane of the nanotubes rope (10, 10) are presented. The calculation was performed for different values of ε_{\perp} (the numbers near trajectories relate to the values of ε_{\perp} in eV). We see that for some values of ε_{\perp} take place the channeling of the particles along the nanotubes axis. Such motion is possible if $\varepsilon_{\perp} < U_c$, where U_c is the value of the potential energy in saddle point. If $\varepsilon_{\perp} > U_c$, then the particle performs infinite (above-barrier) motion with respect to the nanotubes. The particle interacts consequently with different nanotubes in this case.

3. Scattering by single nanotube

We see from Fig. 1(b) that for some cases the particle penetrating inside the nanotube makes a large number of oscillations before it will leave the nanotube. Such motion takes place if $\varepsilon_{\perp} > U_c$. Let us consider this effect in more detail.

During the studies of the particle channeling phenomenon in a nanotube we saw that the azi-

muthal asymmetry of potential leads to a rather complicated particle motion pattern and that a dynamical chaos phenomenon is possible in this case. A similar situation occurs also in the problem of a particle scattering by a nanotube. Therefore, for a determination of the particle trajectory at $\varepsilon_{\perp} \sim U_c$ it is required to numerically solve the two-dimensional equation (2.3).

Some trajectories of positively charged particles in the nanotubes field (10, 0), corresponding to various values of impact parameters, are presented in Fig. 2(a) and (b). The calculations were carried out for $\varepsilon_{\perp} = 75$ eV which is some more then $U_c = 58$ eV in the saddle point. We see that the character of the particle motion essentially depends on the impact parameter in this case. At some values of impact parameter the particle that penetrates inside the nanotube make a large number of oscillations before it will leave the nanotube.

Let us consider the dependence of the time delay of the particle in the space inside the nanotube $T(b)$ from the impact parameter b . Such dependence is presented in Fig. 2(c) and (d).

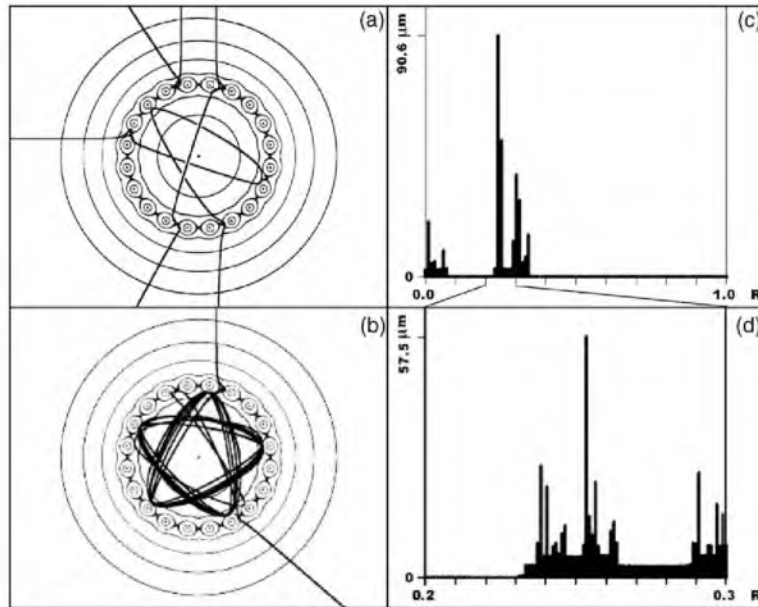


Fig. 2. Trajectories of positively charged particles in a nanotube (10, 0) field (a, b) and dependence $T(b)$ of time delay for positively charged particle in the space inside the nanotube (10, 0) with impact parameter (c, d). The ordinate gives the length $l = T(b) \cdot c$, which the particle passes for the time $T(b)$.

The results show that there are regions of impact parameters in which small changes of impact parameters lead to the considerable changes of the particle scattering. This calculations for Fig. 2(c) were carried out with the step $\Delta b = 10^{-2}\mathfrak{R}$, where \mathfrak{R} is the nanotube radius. Reducing the step of the calculations to the value $\Delta b = 10^{-3}\mathfrak{R}$ we see that for the region of impact parameters where the function $T = T(b)$ changes essentially, the structure of this function does not differ from the initial one. This result is conserved also for subsequent changing of the scale. Such behavior of the function $T(b)$ is called fractal [14].

The analogous situation was discussed in an investigation of the particle scattering by disks [14,15], at scattering by the field of several centers for which the potentials change slowly in space [15–18] and at scattering of the fast charged particles in a crystal [19].

4. Fast particles passage through bent nanotubes

Let us consider now a fast charged particles passage through a bent nanotube rope. Let us show, that in this case, like in the case of the particles passage through a bent crystal (see for instance [19,20]), the beam deflection on the angles, which sufficiently exceed the critical channeling angle is possible.

There are two mechanisms for the beam deflection by bent crystals. One of them is connected with the particle channeling along bent atomic planes of a crystal. The beam deflection is possible in this case if the following condition is fulfilled [19–21]

$$R > R_c = d_p \frac{\varepsilon}{4U_p}, \quad (4.1)$$

where R is the radius of crystal planes bending, d_p is the distance between planes and U_p is the depth of the potential hole, which is formed by continuous planes of the crystal. The other mechanism deals with multiple scattering of particles by bent atomic strings of a crystal. The effective beam deflection is possible in this case if the condition is fulfilled [19,22]

$$R > \psi_c \sqrt{L}, \quad (4.2)$$

where $\psi_c = \sqrt{2U_0/\varepsilon}$ is the critical angle of axial channeling, $U_0 = 2Ze^2/d_r$, $Z|e|$ is the charge of nucleus of a lattice atom, d_r is the distance between atoms in the string, $l \approx d^2/\psi a_{TF}$, d is the distance between atomic strings in crystal and a_{TF} is Thomas–Fermi screening radius for atomic potential. Such conditions can be fulfilled for the beam passage through bent nanotube and nanotubes rope too.

The condition (4.1) means, that the potential hole, inside which the channeling is performed, is not destroyed by the crystal bend. In a nanotube a deep and wide two-dimensional channel is formed. Thus dechanneling of particles in such structure will be smaller than in a crystal. If the radius of a nanotube bending will satisfy the condition (4.1), the bending will not destroy the potential hole and channeled particles will follow the nanotube bend.

Fig. 3 presents simulation results for protons and C^{6+} ions passage through the bent nanotubes rope (10, 10) along the nanotube axis and through the bent diamond crystal along the $\langle 110 \rangle$ axis. A simulation was made with the account of incoherent effects in scattering. The simulation method is the same as for a beam passage through a bent crystal near one of its axes [22]. The simulation results are presented for a set of length that made it possible to retrace the beam deflection dynamics. These results show that for small thickness both of the crystal and nanotube rope the main part of the beam follows the axis bend. In the nanotube rope the beam deflection is mainly caused by channeling effect, while in the crystal the beam deflection is mainly caused by multiple scattering at the bent atomic strings [19,22]. With a thickness growth, due to incoherent scattering, the part of particles, moving infinitely in respect to atomic strings, are captured to the plane channeling regime and follow further along the bend of those planes. Such particles form side branches of angular distributions in Fig. 3. Analogous effect takes place for nanotube rope too, but here it is developed slower.

The dependence of deflected beam fraction upon the target thickness is presented on Fig. 4. As “deflected” we determined those particles of the beam, which are in limits of horizontal angles

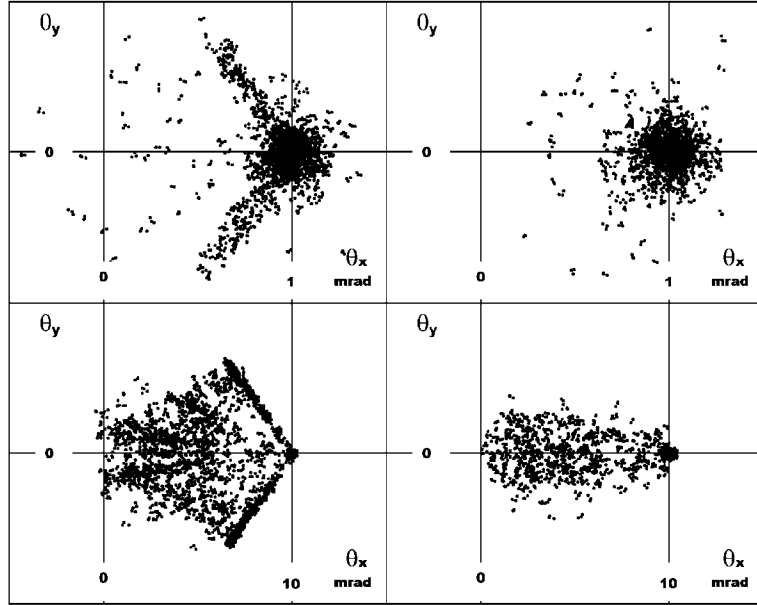


Fig. 3. Angular distributions of C^{6+} ions passing through the bent diamond crystal near the $\langle 110 \rangle$ axis (left pictures) and through a nanotubes (10,10) rope along its axis (right pictures) for different values of target thickness. The beam momentum is $p = 10$ GeV/c, the curvature radius is $R = 20$ cm. Initial direction of the beam and the target axis correspond to $\vartheta_x = 0$, $\vartheta_y = 0$; final direction of the target axis corresponds to $\vartheta_x = 1$ and 10 mrad, $\vartheta_y = 0$. Points are the simulations results. Simulation statistics is 1000 particles.

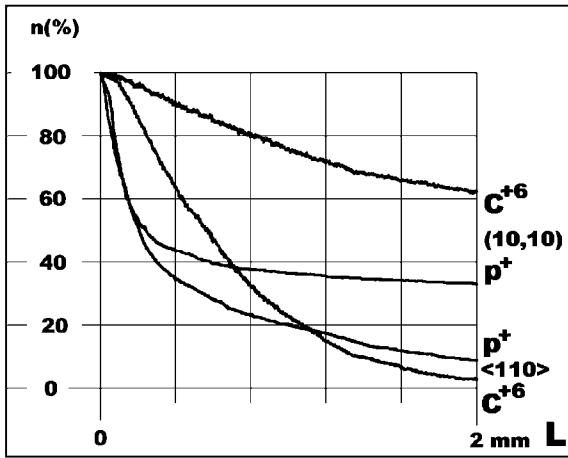


Fig. 4. Dependence of the deflected beam fraction with target length for beam deflection by a bent nanotubes rope and a diamond crystal. The crystal curvature radius is $R = 20$ cm, the beam momentum is $p = 10$ GeV/c. Simulation statistics is 1000 particles.

$-\psi_c < \psi < \psi_c$ respectively to the current direction of the bent axis. A simulation was performed for protons and C^{6+} ions with momentum $p = 10$

GeV/c passing through the bent nanotube rope and the bent crystal.

Simulation results show that in the considered case a beam deflection is possible. In a nanotube rope, beginning from the thickness of order 100 μm , the part of deflected particles decreases slowly with the rope thickness. It deals with the fact, that de-channelling process of ions in this case is caused mainly by incoherent scattering on the electron subsystem of a rope.

Acknowledgements

The work is partially supported by the INTAS project no. 97-30392 and by RFBR project no. 00-02-16337.

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