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# Angular distributions of 1 GeV protons channeled in bent short single-wall carbon nanotubes

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**Abstract**

This study is devoted to the angular distribution of protons of the energy of 1 GeV channeled in a bent short rope of (10, 10) single-wall carbon nanotubes as a function of the bending angle. The rope length was chosen to be 7 μm, corresponding to the reduced rope length associated with the transverse proton motion inside a nanotube equal to 0.103. The bending angle was varied between 0 and 1.5 mrad. The angular distributions of channeled protons and the corresponding rainbow patterns were generated using the theory of crystal rainbows, with the Molière's expression for the continuum potential of the rope. The results obtained show that the total yield of protons channeled in the rope as a function of the bending angle has the inflection point at 0.45 mrad, and that it falls below 10% of the yield for the straight rope at 1.25 mrad.


## 1. Introduction

It has been shown theoretically that in ion transmission through axial channels of very thin crystals the rainbows occur [1]. The approach was via the ion–molecule scattering formalism and it was numerical. In the model the continuum approximation was included implicitly, the correlations between the positions of the atomic strings of the crystal were included, and the assumption of statistical equilibrium in the transverse plane was avoided. The effect has been named the crystal rainbow effect [2]. It has been observed with protons of the energy of 7 MeV transmitted through the $\langle 100 \rangle$ and $\langle 110 \rangle$ Si very thin crystals [3], and with 2–9 MeV protons and 6–30 MeV $C^{q+}$ ions, $q = 4$–6, transmitted through the $\langle 100 \rangle$ Si thin crystals [4].

Krause et al. [4] and Miletić et al. [5–7] showed that evolution of the angular distribution of channeled ions with the reduced crystal thickness had a periodic behavior. The reduced crystal thickness is $\Lambda = f(Q,m)L/V_0$, where $Q$, $m$ and $V_0$ are the ion charge, mass and initial velocity, $L$ is the crystal

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thickness, and $f(Q,m)$ is the frequency of transverse ion motion close to the channel center. The values of variable $\Lambda$ equal to 0, 0.5, 1, ... correspond to beginnings of the cycles of the angular distribution [4], which have been named the rainbow cycles [5]. One says that the crystal is very thin if $\Lambda$ is smaller than 0.25, it is thin if $\Lambda$ is between 0.25 and 1, and it is thick if $\Lambda$ is larger than 1.

Petrović et al. [8] formulated the theory of crystal rainbows, as the generalization of the model of crystal rainbows [1]. It has been demonstrated that the theory enables the full explanation of evolution of the angular distribution of channeled ions with variable $\Lambda$ [8,9].

Carbon nanotubes [10] can be described as sheets of carbon atoms at the (two-dimensional) hexagonal lattice sites rolled up into cylinders [11]. Their diameters are of the order of a nanometer and they can be more than a hundred micrometers long. A nanotube is called a single-wall one if it is formed from one sheet only. Klimov and Letokhov [12] realized that positively charged particles could be channeled in nanotubes. After that, a number of theoretical groups have studied ion channeling in nanotubes [13–17], with the main objective to explore the possibility of guiding high energy ion beams with bent nanotubes. Petrović et al. [17] used the theory of crystal rainbows and revealed that in ion channeling in nanotubes the rainbows occurred. The projectiles were 1 GeV protons and the target was a straight 1 μm long rope of (10, 10) single-wall nanotubes.

## 2. Calculations

We shall report here about the angular distribution of 1 GeV protons transmitted through the bent short (10, 10) single-wall carbon nanotubes as a function of the bending angle. It was assumed that the nanotubes formed a rope whose transverse cross section could be described via a (two-dimensional) hexagonal superlattice with one nanotube per lattice point [18]. The rope length was 7 μm and the bending angle, $\alpha$, was varied in the range of 0–1.5 mrad.

The calculations were performed using the theory of crystal rainbows [8]. The $z$ axis coincided with the rope axis and the origin lay in the entrance plane of the rope. The initial proton velocity vector, $\mathbf{V_0}$, was taken to be parallel to the rope axis. The rope was bent along the y axis. We adopted for the continuum potential of the rope the Molière's expression. The thermal vibrations of the nanotube atoms were taken into account, but the proton energy loss and the uncertainty of the proton scattering angle caused by its collisions with the nanotube electrons were neglected. The bond length of two nanotube atoms was 0.14 nm [11], and, hence, the diameter of a nanotube was 1.34 nm. The distance between the centers of two neighboring nanotubes was 1.70 nm [18]. The one-dimensional thermal vibration amplitude of the nanotube atoms was 0.0053 nm [19].

The nanotube walls define two separate regions in the transverse plane: inside the nanotubes and in between them. Accordingly, the rope is characterized by two types of channels: the circular one, whose center coincides with the center of the region inside each nanotube, and the triangular one, whose center coincides with the center of the region in between each three neighboring nanotubes. The primitive cell of the hexagonal superlattice is a rhomb defined by each four neighboring nanotubes. It is clear that in such a case one has to define two frequencies of transverse proton motion, corresponding to the protons moving close to the centers of the circular and triangular channels. The two frequencies can be determined from the second order terms of the Taylor expansions of the continuum potential of the rope in the vicinities of the centers of the two types of channels. Consequently, there are two reduced rope lengths, $\Lambda_1$ and $\Lambda_2$, corresponding to the proton motions close to the centers of the circular and triangular channels, respectively. In the case we analyze, in which the rope length is 7 μm, $\Lambda_1 = 0.103$ and $\Lambda_2 = 0.488$. Thus, in the circular channels the majority of protons make before leaving the rope less than a quarter of an oscillation around the channel center ($\Lambda_1 < 0.25$), and in the triangular channels they make very close to half an oscillation ($\Lambda_2 \cong 0.5$) [9]. For the protons in the circular channels the rope is very short while for those in the triangular channels it is short ($\Lambda_2 < 1$). This justifies the neglect of the proton energy loss and the uncertainty of the proton scattering angle caused by its collisions with the nanotube electrons. If the rope were long ($\Lambda_1$, $\Lambda_2 > 1$), these effects would cause the smearing out of the angular distributions of channeled protons [20].

## 3. Results

Fig. 1(a) shows the dependence of the yield of protons channeled in the circular channels of the straight rope ($\alpha = 0$) in the region of the scattering angle plane in the vicinity of the origin, i.e. the zero-degree yield of channeled protons, on the rope length in the range of 0–200 μm, comprising the first six rainbow cycles; the $\Lambda_1$ axis is shown too. For the region in the scattering angle plane in the vicinity of the origin we took the region in which variable $\Theta = (\Theta_x^2 + \Theta_y^2)^{1/2}$, where $\Theta_x$ and $\Theta_y$ are the $x$ and $y$ components of the proton scattering angle, respectively, is smaller than 0.0109 mrad. The initial number of protons was 174,976. The six maxima of the dependence correspond to the ends of the first six rainbow cycles, where the proton beam channeled in the circular channels of the rope is quasi-parallel [6,7,9]. Their positions correspond to the values of variable $\Lambda_1$ equal to 0.5, 1, 1.5, ..., and the deviations from these values can be attributed to the anharmonicity of the continuum potential of the rope in the vicinities of the centers of the circular channels [7]. The position of the first maximum of the dependence is $\Lambda_1 = 0.352$.

Fig. 1(b) gives the dependence of the zero-degree yield of protons channeled in the triangular channels of the straight rope on the rope length in the range of 0–200 μm, comprising the first 27 rainbow cycles; the $\Lambda_2$ axis is shown too. The initial number of protons was 136,658. The 27 maxima of the dependence correspond to the ends of the first 27 rainbow cycles, where the proton beam channeled in the triangular channels of the rope is quasi-parallel [6,7,9]. Their positions are close to the values of variable $\Lambda_2$ equal to 0.5, 1, 1.5, ..., and the small deviations from these values can be attributed to the small anharmonicity of the continuum potential of the rope in the vicinities of the centers of the triangular channels [7]. The position of the first maximum of the dependence is $\Lambda_2 = 0.488$. It should be noted that the total

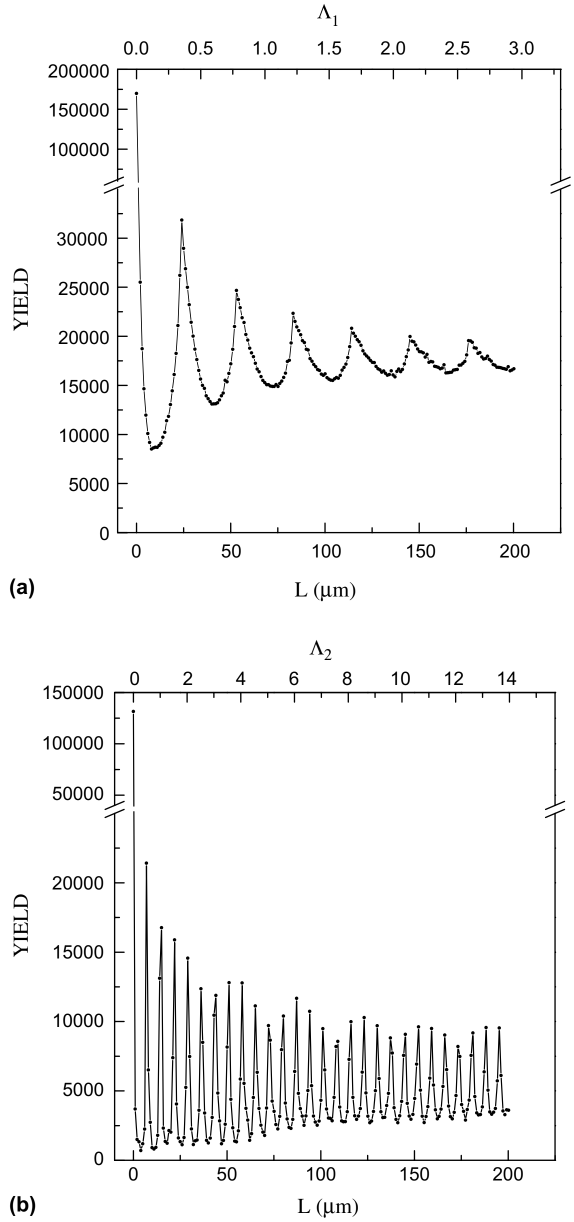


Fig. 1. (a) The zero-degree yield of 1 GeV protons channeled in the circular channels of the straight rope of (10, 10) single-wall carbon nanotubes as a function of the rope length. (b) The zero-degree yield of 1 GeV protons channeled in the triangular channels of the straight rope of (10, 10) single-wall carbon nanotubes as a function of the rope length.

zero-degree yield of protons channeled in the straight rope (both in its circular and triangular channels) as a function of the rope length is the sum of the zero-degree yields shown in Fig. 1(a) and (b).

We can now say that in the case we analyze the rope length was chosen to correspond to the first maximum of the dependence given in Fig. 1(b), i.e. to make the part of the proton beam transmitted through the triangular channels of the rope quasi-parallel, and investigate in an easier manner the behavior of the proton beam transmitted through the circular channels of the rope.

Fig. 2(a) shows the angular distribution of protons transmitted through the rope obtained for variable $\alpha$ equal to zero. The critical angle for channeling is 0.314 mrad. The sizes of a bin along the $\Theta_x$ and $\Theta_y$ axes were equal to 0.00667 mrad while the initial number of protons was 866,976. The angular distribution contains a pronounced maximum at the origin, a non-pronounced circular part and six non-pronounced maxima lying along the lines $\Phi = \tan^{-1}(\Theta_y/\Theta_x) = n\pi/3$, $n$ = 0–5. Fig. 2(b) gives the rainbow pattern in the scattering angle plane for $\alpha = 0$. It contains (i) a circular line, corresponding to a circular line in the impact parameter plane within each circular channel of the rope, (ii) two six-cusp lines very close to the origin, corresponding to two complex lines in the impact parameter plane close to the centers of the two triangular channels making each rhombic channel of the rope [21] and (iii) six points lying along the lines $\Phi = n\pi/3$, $n$ = 0–5, corresponding to two times three points in the impact parameter plane within the two triangular channels making each rhombic channel. The comparison of the results given in Fig. 2(a) and (b) showed that the angular distribution could be explained as follows: the pronounced maximum at the origin was generated by the protons with the impact parameters close to the centers of each circular channel and each triangular channel [21], the non-pronounced circular part by the protons with the impact parameters close to the circular rainbow line (within each circular channel), and the six non-pronounced maxima by the protons with the impact parameters close to the six rainbow points (within each rhombic channel).

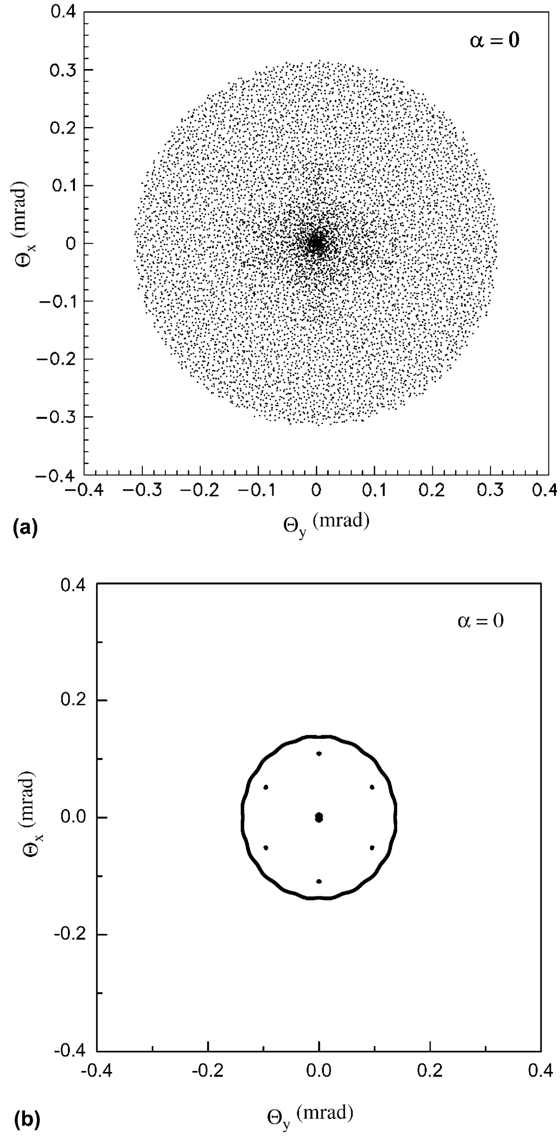


Fig. 2. (a) The angular distribution of 1 GeV protons transmitted through the straight 7 μm long rope of (10,10) single-wall carbon nanotubes. (b) The rainbow pattern in the scattering angle plane of 1 GeV protons transmitted through the straight 7 μm long rope of (10,10) single-wall carbon nanotubes.

Fig. 3(a) shows the angular distribution of protons transmitted through the rope obtained for variable $\alpha$ equal to 0.2 mrad. As in the case of $\alpha = 0$, the sizes of a bin along the $\Theta_x$ and $\Theta_y$ axes were equal to 0.00667 mrad while the initial number

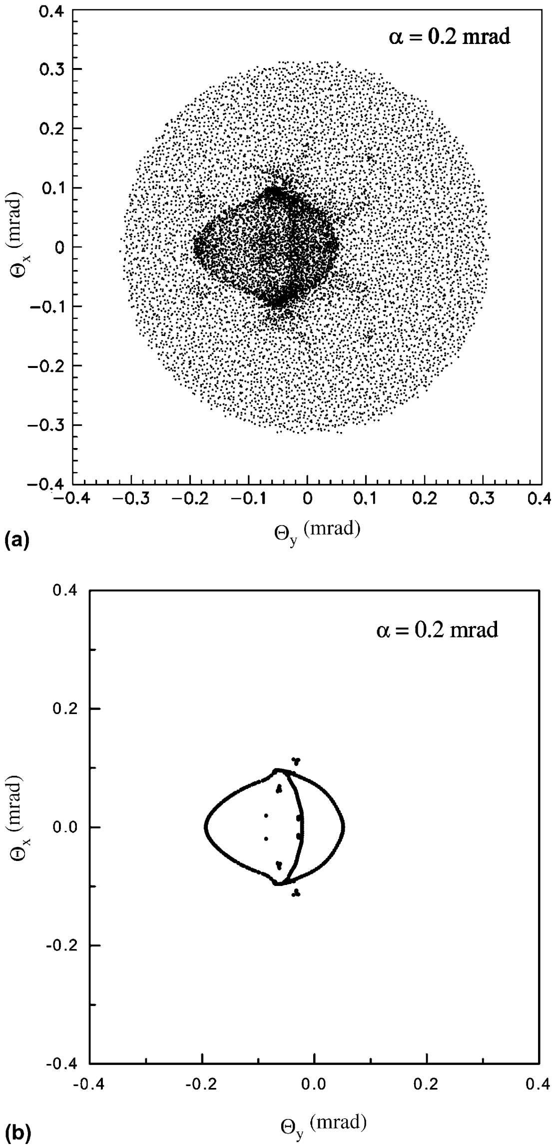


Fig. 3. (a) The angular distribution of 1 GeV protons transmitted through the bent 7 μm long rope of (10, 10) single-wall carbon nanotubes for the bending angle of 0.2 mrad. (b) The rainbow pattern in the scattering angle plane of 1 GeV protons transmitted through the bent 7 μm long rope of (10, 10) single-wall carbon nanotubes for the bending angle of 0.2 mrad.

of protons was 866,976. It must be noted that the scattering angle plane was parallel to the exit plane of the rope. One can see easily that the angular distribution lies in the region $\Theta_y > -0.2$ mrad, demonstrating that the proton beam was bent by the rope effectively. The centrifugal force made the effective bending angle of the proton beam smaller than 0.2 mrad. The angular distribution contains a part having the shape of an acorn with two maxima at points (±0.096 mrad, −0.054 mrad) and eight additional maxima close and in between the two maxima. Fig. 3(b) gives the rainbow pattern in the scattering angle plane for $\alpha = 0.2$ mrad. It contains (i) an acorn-like line with two joining points of its branches, corresponding to a complex line in the impact parameter plane within each circular channel of the rope and (ii) eight groups of points, corresponding to two times four groups of points in the impact parameter plane within the two triangular channels making each rhombic channel of the rope. The comparison of the results given in Fig. 3(a) and (b) showed that the angular distribution could be explained as follows: the acorn-like part with the two maxima was generated by the protons with the impact parameters close to the acorn-like rainbow line with the two joining points (within each circular channel), and the eight additional maxima by the protons with the impact parameters close to the eight groups of rainbow points (within each rhombic channel).

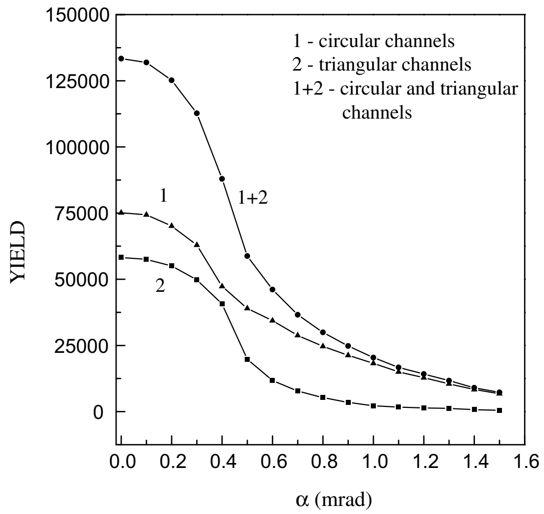


Fig. 4. The yields of protons transmitted through the circular channels, the triangular channels and both the circular and triangular channels of the bent 7 μm long rope of (10, 10) single-wall carbon nanotubes as functions of the bending angle.

Fig. 4 gives the dependences of the yields of protons transmitted through the circular channels and the triangular channels of the rope on variable $\alpha$ in the range of 0–1.5 mrad. The initial numbers of protons were 77,866 for the former dependence and 60,770 for the latter dependence. The inflection points of the dependences appear at $\alpha = 0.35$ and 0.45 mrad, respectively. These values ought to be compared to the value of the critical angle for channeling (0.314 mrad). However, the former yield decreases with $\alpha$ after the inflection point considerably slower than the latter yield. They fall below 10% of the yields for the straight rope at $\alpha = 1.45$ and 0.75 mrad, respectively. The figure also gives the total yield of protons transmitted through the rope (both through the circular and triangular channels) as a function of $\alpha$. Its inflection point appears at $\alpha = 0.45$ mrad, and it falls below 10% of the yield for the straight rope at $\alpha = 1.25$ mrad.

## 4. Conclusions

We have analyzed here the dependence of the angular distribution of 1 GeV protons channeled in a bent 7 μm long rope of (10, 10) single-wall carbon nanotubes on the bending angle, in the range of 0–1.5 mrad. The analysis has been done using the theory of crystal rainbows. Such a rope includes the circular and triangular channels. For the protons moving along the circular channels the rope was very short, and for those moving along the triangular channels it was short. The length of the rope was chosen to make the part of the proton beam transmitted through the triangular channels quasi-parallel, and to investigate in an easier manner the behavior of the proton beam transmitted through the circular channels. The angular distributions of channeled protons have been explained by the corresponding rainbow patterns. For the smaller bending angles the contributions of the circular and triangular channels to the total yield of protons transmitted through the rope are comparable, and for the larger bending angles the contribution of the circular channels dominates the total yield. This can be explained by the fact that the circular continuum potential well is considerably deeper than the triangular one.

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