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AXIAL CHANNELING OF HIGH ENERGY PROTONS IN CARBON NANOTUBES

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Abstract. We have studied theoretically the angular distributions of 1 GeV protons channeled through the long (10, 0) single-wall carbon nanotubes. The nanotube length is varied between 10 and 80 μm. The angular distribution of channeled protons is generated by the computer simulation method using the numerical solution of the proton equations of motion in the transverse plane. The analysis shows that for the nanotube length less then 30μm the transverse geometrical structure of the nanotubes could be deduced from the angular distribution. For the length over 30 μm, the angular distribution is characterized only by the concentric circular ridges. The number of ridges increases and the distance between them decreases as the nanotube length increases. For the nanotube length of 80μm, the circular ridges are no longer visible and the angular distribution becomes equilibrated.

1. INTRODUCTION

Carbon nanotubes were discovered by Iijima in 1991 (Iijima 1991). Soon after nanotubes were discovered, Klimov and Letokhov (Klimov et al. 1996) foresaw the effect of channeling of positively charged particles in them. Petrović et al. applied the theory of crystal rainbows,which has been demonstrated to be the proper theory of ion channeling through thin crystals (Petrović et al. 2000, Nešković et al. 2000) to channeling of 1 GeV protons through the straight and bent (10, 10) single-wall carbon nanotubes (Petrović et al. 2005, Nešković et al. 2005). They showed that the rainbow patterns provide the full explanation of the angular distributions of channeled protons. Recently, in a study of channeling of 0.233 MeV protons through the (11, 9) single-wall carbon nanotubes, Borka et al. demonstrated that the image force acting on the protons gave rise to the additional rainbows in their angular distributions (Borka et al. 2006). Our motivation for the work presented here is to find out how the angular distribution of protons channeled through a (10, 0) carbon nanotube evolves with the nanotube length, and how it looks like when the nanotube is very long.

2. THEORY

The system we investigate is a high energy (relativistic) proton moving through the long (10, 0) single-wall carbon nanotubes. The z axis is taken to be parallel to

nanotube axis and the origin lies in its entrance plane. Each nanotube consists of the straight atomic strings parallel to its axis (Saito et al. 2001). The continuum approximation is assumed (Lindhard 1965), and we use the Molière's expression for the proton-atom interaction potential (Petrović et al. 2000, Nešković et al. 2000, Petrović et al. 2005),

$$V(r) = \frac{Z_1 Z_2 e^2}{r}[0.35exp(-br) + 0.55\exp(-4br) + 0.10\exp(-20br)], \qquad (1)$$

where Z_1 and Z_2 are the atomic numbers of the proton and carbon atom, respectively, e is the elementary charge, r is the distance between the proton and the atom, $b = 0.3/a$, $a = [9\pi^2/(128\,Z_2)]^{\frac{1}{3}} a_0$ is the screening radius, and a_0 is the Bohr radius. The effect of the thermal vibrations of the atoms is included via expression $U_i^{th}(x,y) = U_i(x,y) + (\sigma_{th}^2/2)\,\Delta U_i(x,y)$ where U_i is the continuum potential of the i-th atomic string of the nanotube with the thermal vibrations of the atoms neglected, $\Delta \equiv \partial_{xx} + \partial_{yy}$, x and y are the components of the proton position in the transverse plane, and σ_{th} is the one-dimensional thermal vibration amplitude of the atoms. The continuum potential of the nanotube, U^{th}, is the sum of the continuum potentials of the atomic strings.

For the specific (electronic) proton energy loss we use expression (Gemmell 1974, Petrović et al. 2002)

$$-\frac{dE}{dz} = \frac{4\pi Z_1^2 e^4}{m_e v^2} n_e \left(\ln \frac{2m_e\gamma^2 v^2}{\hbar\omega_e} - \beta^2\right) \qquad (2)$$

where $\omega_e = \left(4\pi e^2 n_e/m_e\right)^{1/2}$ and $n_e = \Delta U^{th}/4\pi$; m_e is the electron mass, v the proton velocity, $\gamma^2 = 1/(1-\beta^2)$, $\beta = v/c$, and c the speed of light; ω_e is the angular frequency of the proton induced oscillations of the electron gas, and $n_e = n_e(x,y)$ is the average (along the z axis) density of the electron gas of the nanotubes. The dispersion of the proton scattering angle due to its collisions with the nanotube electrons is given by expression (Gemmell 1974, Petrović et al. 2002): $\frac{d\Omega_e^2}{dz} = \frac{m_e}{m^2v^2}\left(-\frac{dE}{dz}\right)$, where m is the (relativistic) proton mass. The corresponding standard deviations of the x and y components of the proton scattering angle, Θ_x and Θ_y, respectively, are $\Omega_{ex} = \Omega_{ey} = \Omega_e/\sqrt{2}$. The proton impact parameter is chosen uniformly within the region of the nanotube. For each impact parameter, the x and y components of the initial proton velocity, v_{0x} and v_{0y}, respectively, are chosen within the Gaussian distributions with the standard deviations $\Omega_{bx} = \Omega_{by} = \Omega_b/\sqrt{2}$, where Ω_b is the divergence of the proton beam.

3. RESULTS AND DISCUSSION

We study here the angular distributions of 1 GeV protons channeled through the long (10,0) single-wall carbon nanotubes. The length is varied between 10 and 80 μm. Since the bond length of two carbon atoms is 0.14 nm, the radius of a nanotube is 0.39 nm and the thickness of one atomic layer is 0.21 nm (Saito et al. 2001). The one-dimensional thermal vibration amplitude of the atoms is estimated, using the Debye approximation, to be 0.0053 nm (Hone et al. 2000). The initial number of protons is 5 000 000. The divergence of the proton beam is set at $\Omega_b = 0.1\Psi_c$ mrad, where $\Psi_c =$

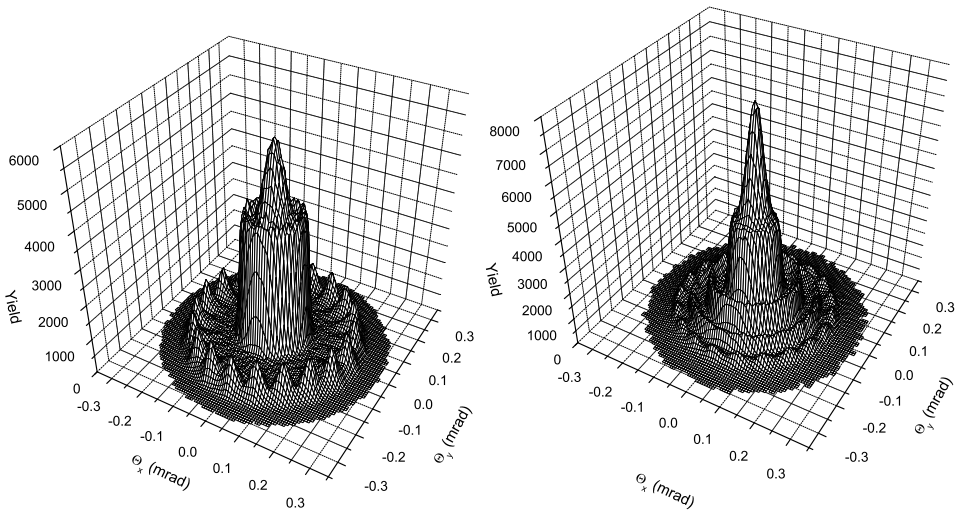

Figure 1: The angular distributions of 1 GeV protons channeled through the (10, 0) single-wall carbon nanotube of the length of 10 μm (*left panel*) and 30 μm (*right panel*).

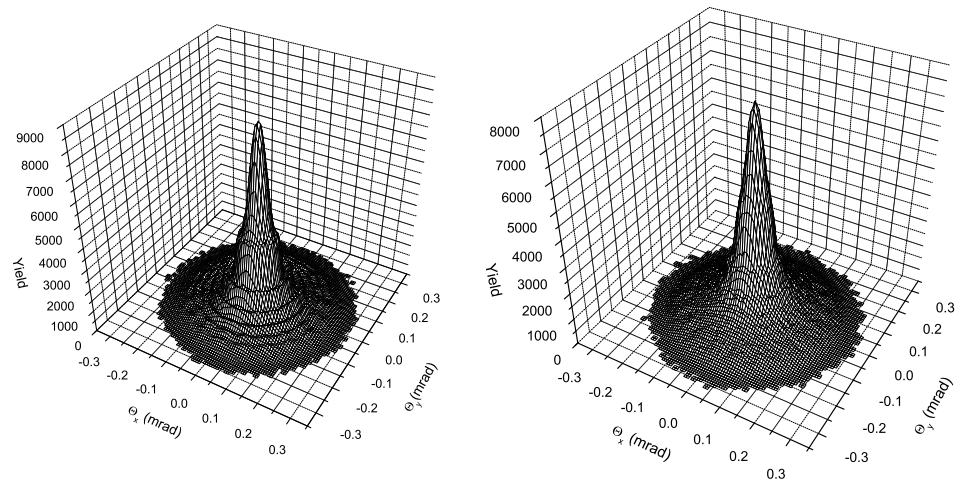

Figure 2: The same as in Fig. 1, but for 50 μm (*left panel*) and 80 μm (*right panel*).

0.0314 mrad is the critical angle for channeling. The proton whose impact parameter happens to be inside one of the circles around the atomic strings of the radius equal to the screening radius is treated as if it is backscattered and is disregarded.

Fig. 1 (left panel) shows the angular distribution of 1 GeV protons channelled through the (10, 0) single-wall carbon nanotube, in the case of nanotube length $L =$ 10 μm. It is characterized by 20 maxima lying on the lines $\Phi = \arctan(\Theta_y/\Theta_x) = (n+1)\pi/10$, $n =$ 0-19, in the peripheral region of the scattering angle plane, one

concentric circular ridge in the central region of the scattering angle plane and the maximum at the origin. The appearance of the 20 maxima is connected to the symmetry of the transverse geometrical structure of the nanotube, which consists of 20 atomic string parallel to the nanotube axis (Saito et al. 2001). For $L = 30$ μm, the angular distribution of 1 GeV protons channelled through the (10, 0) single-wall carbon nanotube is shown in Fig. 1 (right panel). It is characterized by 20 maxima lying on the lines $\Phi = (n+1)\pi/10$, n = 0-19, in the peripheral region of the scattering angle plane, two concentric circular ridge in the central region of the scattering angle plane, and the maximum at the origin. It is clear that the transverse geometrical structure of the nanotube could be deduced from the angular distribution.

Fig. 2 (left panel) shows the angular distribution of 1 GeV protons channelled through the (10, 0) single-wall carbon nanotube, in the case of $L = 50$ μm. One can see that it is characterized by the five concentric circular ridges, and the maximum at the origin. One ridge lies in the peripheral region and the others in the central region of the scattering angle plane. Clearly, the transverse geometrical structure of the nanotube is no longer visible in the angular distribution. It should be noted that the ridges are closer than in the previous case ($L = 30$ μm). Also, the analysis shows that the observed trend in the angular distributions i.e. the increase of the number of concentric ridges and decrease of the average distance between them as variable L increases also holds for $L > 50$ μm. Finally, for $L = 80$ μm, the angular distribution of 1 GeV protons channelled through the (10, 0) single-wall carbon nanotube is shown in Fig. 2 (right panel). The angular distribution is a bell-shaped one with no longer visible circular ridges structure. Hence, the angular distribution becomes equilibrated.

The results presented here indicate how the angular distribution of channeled protons through carbon nanotube could be used for its characterization. Namely, each nanotube presumably has its characteristic pattern of the concentric circular structures in the angular distributions of the channeled protons. Additional way to experimentally distinguish between different nanotubes would be to measure the change of the patterns of concentric circular structures in the angular distributions by changing the proton energy, which is equivalent with the change of nanotube length analyzed here.

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