Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Channeling of protons through radial deformed carbon nanotubes

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ARTICLE INFO

Article history:
Received 27 December 2016
Received in revised form 14 February 2017
Accepted 17 March 2017
Available online xxxx
Communicated by R. Wu

Keywords:
Carbon nanotubes
Channeling
Radial deformation

ABSTRACT

In this paper we have presented a theoretical investigation of the channeling of 1 GeV protons with the radial deformed (10, 0) single-wall carbon nanotubes (SWNTs). We have calculated channeling potential within the deformed nanotubes. For the first time we presented theoretically obtained spatial and angular distributions of channeled protons with radially deformed SWNT. We used a Monte Carlo (MC) simulation technique. We show that the spatial and angular distributions depend strongly of level of radial deformation of nanotube. These results may be useful for nanotube characterization and production and guiding of nanosized ion beams.

1. Introduction

After the discovery of the carbon nanotubes (CNT) in 1991 by Sumio Iijima at the NEC Fundamental Research Laboratory in Tsukuba [1], many theoretical groups have attempted to explain ion channeling in CNT [2–27]. At the very beginning of theoretical consideration of charged particle channeling in CNT, Klimov and Letokhov [2] predicted that they could be used to channel positively charged particles. Theoretical modeling of ion channeling in MeV energy range through CNT (where dynamic polarization of nanotube electrons play important role) have been reported by Mišković and coauthors [8,16–18,21]. Detailed discussion about the influence of the nanotube diameter on the channeling high energy ion beams has been performed by Biryukov and Bellucci [6,10]. Also, Krasheninnkov and Nordlund [9] performed a series of molecular dynamics simulations to investigate motion of low energy Ar^+ ions through achiral and chiral CNT. Petrović and coworkers successfully explained spatial and angular distributions of channeling protons through SWNT using theory of crystal rainbows [12]. The investigation of interactions of charged particles with CNT is of reasonable importance since it allows elucidating a possibility of guiding ion beams with CNT. Experimental evidence of ion channeling through CNT also has been reported. Direct experimental confirmation of He^+ ions of the energy of 2 MeV channeling through CNT is obtained by Zhu et al. [28]. Furthermore, Chai et al. [29] experimentally verified that aligned nanotubes of the length in a range of 0.7–3 μm allow transport of 300 keV electrons.

It has been shown that carbon nanotubes may undergo changes in its geometrical structure. Radial deformation can appear under external mechanical stress [30,31] or external electric field [32,33]. Radial deformation is permanent defect occur in carbon nanotubes. For example it has been shown that using an atomic force microscope, CNTs can be radially deformed [32]. Radial deformation of carbon nanotubes has also attracted much attention because of its possible influence on the mechanical and electronic properties [30–33]. The presence of defects and deformations might have large influence of nanotube's channeling properties and it is worth to investigate this influence. The channeling potential in deformed SWNTs has been recently investigated by Abu-Assy and Saliman [34].

In the present work we investigated transmission of 1 GeV incident protons through a straight radially deformed SWNTs of length of few μm, so the influence of the nanotube edges are not included in MC calculations of the spatial and angular distributions. We chose the nanotube length of 1 and 3 μm to have the target that could be made using the existing techniques. Then, we chose the ion species and energy (protons of 1 GeV), to have the projectiles that can be delivered routinely using the existing accelerators and to make the nanotube very short. Using this proton energy we have to include the relativistic effect in its equations of motion, i.e., we had to perform the calculations with the proton mass corresponding to this energy, which is larger than its rest mass. For the first time we presented theoretically obtained spatial and angular distributions of channeled protons with radially deformed SWNT.

This paper is organized as follows. In Section Theory we briefly explained the process of ion channeling in CNT. In Section Results and discussion we presented the contour plots of the channel-

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http://dx.doi.org/10.1016/j.physleta.2017.03.029
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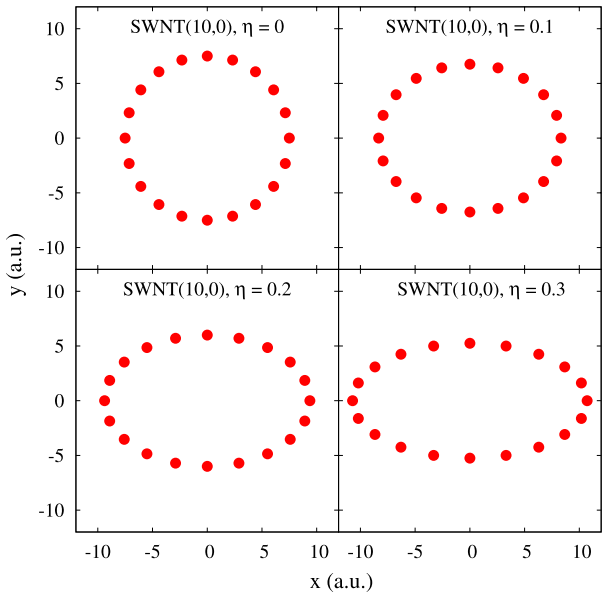

Fig. 1. The view along axes of short (10, 0) SWNTs under different radial strains: (left top) $\eta = 0$ (perfect nanotube); (right top) $\eta = 0.1$; (left down) $\eta = 0.2$; (right down) $\eta = 0.3$, respectively.

ing potential, and the spatial and angular distributions of protons channeling through radial deformed SWNT. It should be noted that all results were obtained using a MC simulations. Finally, the concluding remarks are given in Section Conclusions and perspectives.

2. Theory

This paper consider the SWNTs as a straight cylinder with a circular or elliptical cross-section, depending on whether the radial deformation doesn't exist or exist, respectively and with N atomic rows (for example $N = 20$ in Fig. 1). The spatial and angular distributions for relativistic protons of 1 GeV channeled in the (10, 0) SWNT, has been calculated. For convenience, the z-axis of the right Cartesian coordinate system is chosen so that it coincides with the axis of the SWNTs, with the beginning of which is located in the entry plane of protons into the nanotubes. Proton initial velocity is along $-z$ direction. The length L of the nanotubes which will be discussed here are in the range of few μm so taking into account the ratio between the protons velocity and the length of SWNTs, the energy loss of channeled protons become negligible. Also, we can neglect dynamic polarization effects of carbon nanotube valence electrons because these effects becomes important for proton energy less then 5 MeV [35,36].

A classical approach can be used to consider interaction of the proton and a carbon nanotube atoms [37]. A 1 GeV proton has a velocity of $v = 120.0474$ a.u. ($c = 137.0355$ a.u.), a rest mass of $m_0 = 1822.9$ a.u., a relativistic mass of $m_r = 3779.97$ a.u. and a wavelength $\lambda = 0.000013846$ a.u. $= 7.3271 \times 10^{-7}$ nm. Since λ is much smaller than the bond length between nanotube atoms (0.144 nm) [38], we treat this problem classically. The proton motion in the transverse plane is non-relativistic, the corresponding equations of motion are made relativistically correct by using the relativistic proton mass instead of its rest mass [6,11,39]. Transverse motion of protons can be treated classically for much lower energies then in our paper [40]. Even for electron (positron) energies about 10 MeV it becomes possible to use classical mechanics [11]. Because the number of transverse states in the axial potential wells grows approximately linearly with the particle energy E and for electron (positron) energies about 10 MeV it becomes possible to use classical mechanics for the description of the transverse motion [11]. Also, similar analysis of motion of charged particles are considered as quantum or classical in papers [4,37]. In case of charged particles of much lower energies quantum approach should be applied [11,41,42].

Let $x(t)$ and $y(t)$ are the horizontal and vertical component of a moving proton at the moment t in the transverse plane, respectively. In order to determine appropriate distributions of transmitted protons, it is necessary to solve the following equations of motions:

$$m_r \frac{d^2x(t)}{dt^2} = -\frac{\partial U(x,y)}{\partial x}, \quad x(0) = x_0, \quad \frac{dx(t)}{dt}\Big|_{t=0} = 0 \tag{1}$$

$$m_r \frac{d^2y(t)}{dt^2} = -\frac{\partial U(x,y)}{\partial y}, \quad y(0) = y_0, \quad \frac{dy(t)}{dt}\Big|_{t=0} = 0 \tag{2}$$

where $m_r = m_0/\sqrt{1-(v/c)^2}$ is the relativistic proton mass and m_0 is its rest mass, v is the intensity of the velocity vector of the proton with initial condition $dz(t)/dt \approx v$ for $t = 0$ (a moment of entrance of the proton into carbon nanotubes), and c denotes the speed of light. Taking into account the continuum model approximation [43], the proton nanotube interaction potential $U(x, y)$ which appears in Eqs. (1) and (2) can be expressed through the Molière's approximation of the Thomas–Fermi interaction potential [44] $V(r)$, as a function of the proton–atom distance r, in the following form:

$$U(x,y) = \sum_{k=1}^{J} \frac{1}{d} \int_{-\infty}^{\infty} V\left(\sqrt{\rho_k^2 + z^2}\right) dz \tag{3}$$

where the k-th term in the sum represents the continuum interaction potential of the proton and the k-th atomic string, with the distance d between average centers of two adjacent carbon atoms along the row, while the ρ_k is the distance between the proton and k-th string. The total number of atomic strings in the SWNTs is indicated by J. The position of each proton at the entrance (x_0, y_0) is chosen randomly from a uniform distribution within the cross-sectional area of the entrance plane of the carbon nanotube.

Regardless of whether the small deformation of the nanotubes takes place as a result of the mechanical stress or due to the presence of electric field, the intersection of the nanotube with the transverse plane gives an ellipse with semi-major axis R_x and semi-minor axis R_y [32]. On the other hand, the semi-axis can be expressed as a function of the radius R of the undeformed SWNT and the parameter η that defines the level of radial deformation in the form of $R_x = R(1-\eta)^{-1}$ and $R_y = R(1-\eta)$. The radial cross section of the nanotube can take different forms in case of different degree of radial deformation. It has been found experimentally that when the applied strain $\eta < 0.35$, the radial cross-section of the nanotube has an elliptical-like shape [32,34].

In this paper, emphasis will be placed precisely on the consideration of relatively small radial deformation, i.e., for three cases $\eta = 0.1$, 0.2 and 0.3. The chiral index (n, m) together with interatomic length l (the bond length between carbon atoms ≈ 0.144 nm), uniquely determined the value of the radius R by $R = l\sqrt{3}(2\pi)^{-1}\left(n^2 + nm + m^2\right)^{1/2}$. Finally, if the position of the carbon atom of the k-th atomic string in a plane perpendicular to the nanotube axis is determined by the angle $\theta_k = \arctan\left(\frac{R_y}{R_x}\tan\left(2\pi(k-1)/N\right)\right)$ relative to the semi-major axis and the distance from the center of the SWNT $R_k = \left(R_x^{-2} - \sin^2\theta_k\left(R_x^{-2} - R_y^{-2}\right)\right)^{-1/2}$ [34], the interaction potential can be represented in the following form:

Please cite this article in press as: V. Borka Jovanović et al., Channeling of protons through radial deformed carbon nanotubes, Phys. Lett. A (2017), http://dx.doi.org/10.1016/j.physleta.2017.03.029