Nuclear Instruments and Methods in Physics Research B xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Channeling of protons in radially compressed chiral carbon nanotubes

A. Karabarbounis [a], S. Sarros [a,*], Ch. Trikalinos [b]

[a] Department of Physics, Section of Nuclear and Particle Physics, National and Kapodistrian University of Athens, Panepistimioupolis, Ilissia, 15771 Athens, Greece
[b] Department of Philosophy and History of Science, National and Kapodistrian University of Athens, Panepistimioupolis, Ilissia, 15771 Athens, Greece

ARTICLE INFO

Article history:
Received 16 November 2016
Received in revised form 5 March 2017
Accepted 6 March 2017
Available online xxxx

Keywords:
Channeling
Nanotubes
Radial compression
Angular distribution

ABSTRACT

Channeling of 10 MeV protons in various types of point and area radially compressed chiral carbon nanotubes (CNTs) is considered. Monte Carlo simulation program is used for the calculation of the trajectories, energy losses and angular distributions of protons in (6,4) and (11,9) CNTs of 2000 nm length, where the potential in Doyle-Turner approximation is used to describe the interaction between a proton and a nanotube. Carbon nanotubes, which are considered, are radially compressed at two points (500 nm and 1500 nm each), at a middle area of various lengths, at three points (both ends and at the centre) and at both ends with a middle area remaining uncompressed. The results show that in a specific case of compressed nanotube a decreased angular distribution of the beam is observed, compared even with propagation in a straight uncompressed nanotube. Furthermore, the energy distribution of channeled protons depends on the type of compression.

1. Introduction

The discovery of carbon nanotubes (CNTs) [1–3] and the considerable progress that has been achieved on the investigation of their unique physical properties and production methods, has given a significant boost on various applications in nanoelectronics, nanomechanics and other fields [4–6]. Another field were possible applications of CNTs are examined, is guidance and beam shaping of high and low energy charged particles beams. One of the main effects that is examined during guidance of charged particle beams in CNTs is channeling. Channeling effect of charged particles in crystals has been studied theoretically and experimentally for many years, and lately many theoretical works are devoted to channeling of charged particles in straight or bent carbon nanotubes with ideal structure [7,8]. In order to simulate more realistic situations, it is necessary to investigate propagation of charged particles in carbon nanotubes with less ideal structure. One deformation of nanotubes can be a radial compression [9] and channeling of protons in such structures has been investigated in our previous works [10,11], were we have shown that such compressed nanotubes may provide a suitable geometrical structure for particle focusing. Another deformation which has been also studied recently is that of random curvature of a nanotube [12]. In present work we propose new geometrical structures of carbon nanotubes, which may approach realistic ones and also may provide better focusing of the beam. Specifically, we investigate the cases when CNT has point compression at different points and when CNT is compressed at a whole area.

2. Theory

It is well known [7,8] that each carbon nanotube can be described by two indices as (n, m) and it may be considered as a collection of atomic rows parallel to the axis of the nanotube and arranged in a specific way along the perimeter of the cylindrical surface. Thus, each pair of these indices define the nanotube radius R and helicity or chiral angle θ:

$$R = (l\sqrt{3}/2\pi)\sqrt{n^2 + nm + m^2} \quad (1)$$

$$\theta = \arctan[\sqrt{3}m/(m + 2n)] \quad (2)$$

where $l = 0.142nm$ is the length of the bond between the carbon atoms [4,5]. Single wall carbon nanotubes (SWCNTs) with $m = 0$ ($\theta = 0^\circ$) are called zigzag, those with $m = n$ ($\theta = 30^\circ$) are called armchair, and all the others ($0^\circ < \theta < 30^\circ$) are called chiral. In the present study we examine only the case of chiral nanotubes.

Considering the motion of fast positively charged particles (e.g. protons) in a straight isolated carbon nanotube, in the case when each such particle enters the nanotube at small enough angle θ_0 with respect to its axis, then it is governed by the continuum potential, i.e. the actual periodic potential of the rows averaged over the direction parallel to the rows. Applying the concept of

* Corresponding author.
E-mail address: stsarros@phys.uoa.gr (S. Sarros).

http://dx.doi.org/10.1016/j.nimb.2017.03.023
0168-583X/

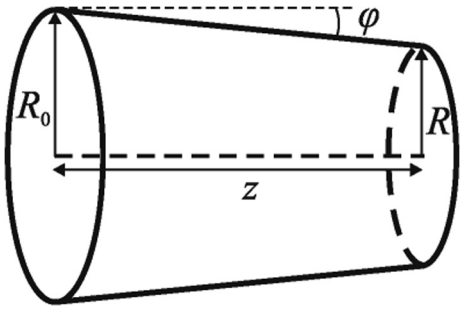

Fig. 1. Geometrical structure of a carbon nanotube radially compressed at one end.

continuum potential to chiral nanotubes, it can be considered as the continuum potential of the (rolled-up) graphite plane, and thus we may average the actual potential of a nanotube over the circumference, i.e. the azimuthal angles. In the Doyle-Turner approximation to the atomic form-factor, the axially symmetrical continuum potential of a chiral nanotube (without taking into account the thermal vibrations of the atoms) can be described by the following expression [7]:

$$U(r,\varphi) = 3^{-3/2}32\pi Ze^2L^{-2}R\sum_{j=1}^{4}\alpha_j b_j^2 \exp[-b_j^2(r^2+R^2)]I_0(2b_j^2Rr) \quad (3)$$

where $Z = 6$ is the atomic number of the carbon atom, r is the distance from nanotube axis and α_j, b_j are dimensional parameters in the Doyle-Turner approximation:

$$\{\alpha_j\} = \{3.222, 5.270, 2.012, 0.5499\} \times 10^{-4}\text{nm}^2$$

$$\{b_j\} = \{10.330, 18.694, 37.456, 106.88\}\text{nm}^{-1}$$

In case of a nanotube that is radially compressed at one end or at random point, its radius at each transverse plane at a point z of the axis is defined as:

$$R = R_0 - z \cdot \tan\varphi \quad (4)$$

where R_0 is the radius of the uncompressed nanotube and φ is the angle of the slope of the walls of the nanotube after compression (see Fig. 1). This way, by introducing Eq. (4) into (3) instead of R, we can obtain the potential in this compressed nanotube. The above approach is valid, since we consider small radial compression of the nanotube, so that the geometry of the nanotube doesn't change significantly and therefore we can use the same expressions for the nanotube potential. In present work we consider 10 MeV protons incident to nanotubes with different types of compression.

As was proved by Lindhard [13] and explained by Thompson [14] in case of channeling of particles with mass greater that the mass of electrons, such as protons, we can always use classical approach because the transverse de Broglie wavelength $\lambda_\perp = \lambda_D/\sin\theta_0$ (see also [7]) of them is always very small compared with channel width. We use the right-handed Cartesian coordinate system for the geometry of our problem, where z-axis coincides with the axis of the nanotube and x, y axes lie on the transverse plane ($r = \sqrt{x^2+y^2}$) and as initial conditions we consider coordinates (x,y) of the point of incidence, the angle between incident proton beam and the nanotube axis, and the angular deviation of the beam. Equations of motion then can be calculated from Newton's second law as:

$$m_1\frac{d^2\mathbf{r}}{dt^2} = -\left(\frac{\partial U(x,y,z)}{\partial x}\hat{\mathbf{i}} + \frac{\partial U(x,y,z)}{\partial y}\hat{\mathbf{j}}\right) \quad (5)$$

where m_1 is the proton mass and as initial conditions we consider coordinates (x,y) of the point of incidence, the angle between incident proton beam and the nanotube axis, and the angular deviation of the beam.

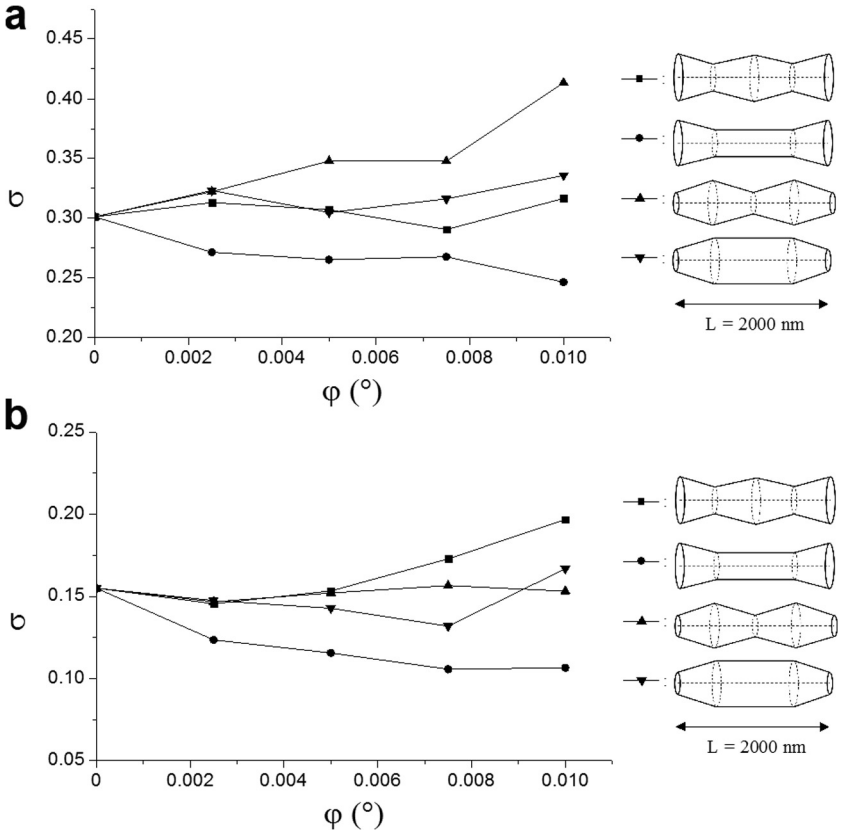

Fig. 2. Standard deviation of angular distribution for theta-x section profile vs. angle of wall slope of various types of radially compressed (6,4) (a) and (11,9) (b) CNTs.

Please cite this article in press as: A. Karabarbounis et al., Channeling of protons in radially compressed chiral carbon nanotubes, Nucl. Instr. Meth. B (2017), http://dx.doi.org/10.1016/j.nimb.2017.03.023