Nuclear Instruments and Methods in Physics Research B xxx (2015) 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 various types of radially compressed carbon nanotubes

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

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

ARTICLE INFO

Article history:
Received 29 November 2014
Received in revised form 4 March 2015
Accepted 6 March 2015
Available online xxxx

Keywords:
Channeling
Nanotubes
Energy loss

ABSTRACT

Channeling of 10 MeV protons in various types of radially compressed chiral carbon nanotubes is considered. Monte Carlo simulation program is used for the calculation of the trajectories, energy losses and angular distributions of protons in nanotubes of various lengths, 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 the centre or at both ends. The results show that in some cases a decreased angular distribution of the beam is observed, compared with propagation through a straight nanotube. Furthermore, the energy distribution of channeled protons in nanotubes present a series of small peaks besides a main one, the number of which depends on the nanotube length and the angle of incidence, which in some cases are significantly high.

1. Introduction

Since the discovery of carbon nanotubes more than twenty year ago [1–3] a considerable progress on the investigation of their properties and production methods has been achieved. Due to their unique physical properties, carbon nanotubes (CNTs) have attracted growing interest on various applications in nanoelectronics, nanomechanics and other fields [4–6]. Carbon nanotubes are produced with various radii and in a wide range of lengths (up to several μm and even mm).

One of possible applications of carbon nanotubes in the field of high and low energy charged particles beams is their guidance using CNTs. 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 for many years (see for example [7]), and lately even in laser fields [8]. Theoretical investigation of charged particles channeling in CNTs has produced several interesting results [9–11], which concern straight nanotubes. Recent studies have shown that they can undergo axial and radial compression [12], and this way it is feasible to obtain carbon nanotubes that are radially compressed at one end, that will resemble truncated nanocones. In our recent study [13] we have shown that compressed carbon nanotubes at one end provide a suitable geometrical structure for particle focusing. New geometrical structures for particle focusing could be obtained by combining such radially compressed CNTs, and it is interesting to investigate the propagation and channeling of protons in such structures.

2. Theory

Each 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. This way, from simple geometrical consideration, each pair of these indices define the nanotube radius R and helicity or chiral angle θ (in practice, the angle under which the most closely packed rows of carbon atoms are wound on the cylindrical surface of the tube):

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

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

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

Let us first consider the case of motion of fast positively charged particles (e.g. protons) in a straight isolated carbon nanotube. If

* Corresponding author. Tel.: +30 6978762212.
E-mail address: stsarros@phys.uoa.gr (S. Sarros).

http://dx.doi.org/10.1016/j.nimb.2015.03.019
0168-583X/© 2015 Elsevier B.V. All rights reserved.

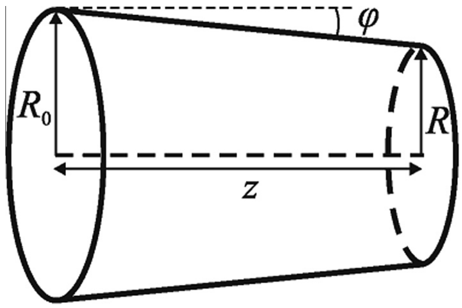

Fig. 1. Geometrical structure of a carbon nanotube radially compressed at one end.

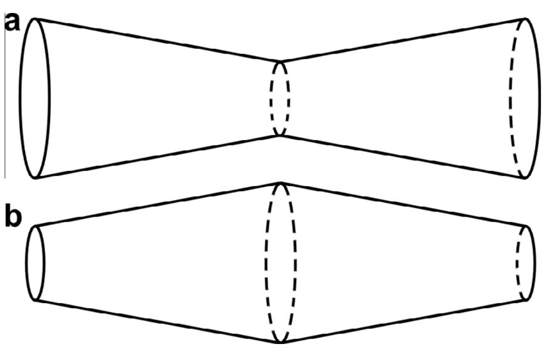

Fig. 2. Geometrical structure of a carbon nanotube radially compressed: (a) at the centre and (b) at both ends.

such a particle enters a single crystal at small enough angle θ_0 with respect to an atomic row, 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 [7]. Applying the concept of 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 [9]:

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

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:

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

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

It should be noticed that Eq. (3) is valid not only inside a nanotube, but outside it as well.

In case of a nanotube that is radially compressed at one end, 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 does not change significantly and therefore we can use the same expressions for the nanotube potential.

If we combine two radially compressed carbon nanotubes, then we can obtain various types of compressed CNTs, and particularly we examine two cases: a CNT compressed at the centre of the axis and a CNT compressed at both ends (see Fig. 2a and b).

Because the de Broglie wavelength of a 10 MeV proton under consideration is very small compared with atomic dimensions,

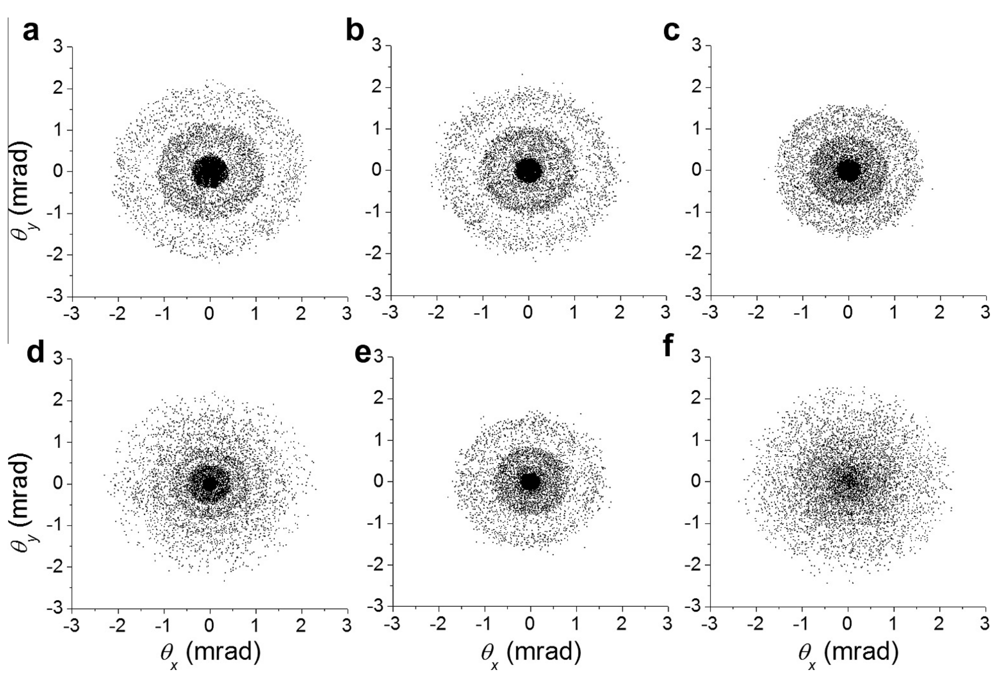

Fig. 3. Angular distribution of well collimated ($\Delta\theta = 0$) 10 MeV protons with zero incident angle channeled in a (6,4) CNT of 1000 nm length in cases of proton incident at: (a) straight, (b) compressed at the end, (c) compressed at the entrance nanotube, and for CNT of 2000 nm length in cases of proton incident at: (d) straight, (e) compressed at the centre, (f) compressed at both ends nanotube. Angle of wall slope in compressed nanotubes is 0.005° (0.087 mrad).

Please cite this article in press as: A. Karabarbounis et al., Channeling of protons in various types of radially compressed carbon nanotubes, Nucl. Instr. Meth. B (2015), http://dx.doi.org/10.1016/j.nimb.2015.03.019