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Channeling of high-energy particles in a multi-wall nanotube

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Abstract

Channeling of high-energy particles in straight and bent multi-wall nanotubes (MWNT) has been studied in computer simulations and compared to the channeling properties of single-wall nanotubes (SWNT) and bent crystal lattices. It is demonstrated that MWNT can efficiently channel positively-charged high-energy particles trapped between the walls of MWNT. Bending dechanneling in MWNT has been computed as a function of the particle momentum to nanotube curvature radius ratio, pv/R. It is found that a bent MWNT can steer a particle beam with bending capabilities similar to those of bent silicon crystal lattice and to those of best (i.e., the narrowest) SWNT. In view of channeling applications at particle accelerators, MWNT appear favored as compared to SWNT, because MWNT can be produced quite straight (and in aligned array), while SWNT is typically very curved, thus posing a severe problem for channeling applications. Therefore, we suggest that MWNT provide a better candidate for channeling than SWNT.

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1. Introduction

Bent channeling crystals are well established as a technical tool for steering of particle beams at accelerators [1]. The related physics has been experimentally tested in the energy range spanning over six decades, from 3 MeV [2] to 900 GeV [3,4]. Today, bent crystals are broadly used for extraction of 70-GeV protons at IHEP (Protvino) with efficiency of 85% routinely obtained at intensity well over 10¹² particle per sec-

ond [5]. Channeling technique is used at IHEP for beam delivery since 1987 on everyday basis [6,7]. About ten channeling crystals are installed on six locations in the main ring of the 70 GeV proton accelerator of IHEP. A bent crystal (5 mm Si) was installed into the Yellow ring of the Relativistic Heavy Ion Collider where it channeled Au ions and polarised protons of 100–250 GeV/u, within the framework of the collimation experiment [8]. There has been interest to apply channeling technique at accelerators from TeV colliders for collimation and extraction [9–12] down to sub-GeV microbeam facilities [13], or, for instance, to use it for a channeling undulator [14–16].

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Nanostructured material offers an interesting alternative to crystal lattices as a guide for channeled particles [17,18]. First, it is a material with very unusual properties [19]. The channels in the nano-ordered material can be much wider than those in crystals, and the channeled particles are trapped in two dimensions (in a nanotube) rather than in one dimension like with crystal planar channels. Second, the nano-material can be designed to fit applications the best, in principle, with a wide choice of geometrical characteristics and atomic content [19,20].

Single-wall nanotube (SWNT) channeling has been studied in computer simulations by several authors [17, 21–23]. In our previous simulation study [24] of channeling in straight and bent SWNT we answered the question of what kind of nanotube geometry (diameter) would fit best the application of SWNT for particle beam steering at accelerators. Another essential question answered [24] was: how SWNT compares to bent crystal lattice in particle channeling. Narrow (order of 1 nm in diameter or less) nanotubes were found to have an efficiency of beam bending similar to that of silicon crystal lattice, while wider nanotubes appear useless for particle steering because of poor efficiency [24].

Multi-wall nanotubes (MWNT) have not been a subject of channeling research so far. While SWNT with its wide channel looks at first glance a naturally attractive object for channeling research, MWNT is a rather dense pack of walls with the spacing of about 0.34 nm (in the case of carbon) which is much narrower than the width of SWNT. However, it is still about two times larger than the spacing in the crystal lattice channels. MWNT are a very common nanostructure and actually were discovered first, ahead of SWNT.

An essential feature of MWNT is that it is very straight on production, unlike SWNT which is very curved. Also, MWNT are much more easily produced as an aligned array of straight parallel tubes than SWNT. From the practical viewpoint of channeling applications all this is of paramount importance. However, the channeling properties of MWNT have to be demonstrated first and clarified. Further on, the fact found in the study [24] that the spacing in the channel should not be too large, in order to make it efficient has also stimulated us to try MWNT for channeling. Finally, without Monte Carlo simulation of a particle beam interaction with a nanostructure, it is very difficult to decide what kind of nanostructure would be best suited for channeling.

2. Channeling in MWNT

For Monte Carlo simulations of particle interaction with a MWNT we applied the same model as in our previous work [24] on SWNT channeling. The model was upgraded to take into account multiple walls. A MWNT has an internal diameter (the one of the narrowest tube in the pack) and an external diameter. Their typical values are a few nanometers and a few tens of nanometer respectively, for carbon nanotubes [19,20].

Channeling inside the internal diameter of MWNT is not of interest, because of poor efficiency shown due to a large width of this channel [24] and because of its small cross-section with respect to the total crosssection of the MWNT. Therefore, we were interested in channeling between the walls in the bulk of MWNT. Our simulations were done for carbon MWNT.

As previously, we average the potential $U(\rho, \phi, z)$ of a straight nanotube over the longitudinal coordinate z and azimuth angle ϕ to obtain a potential $U(\rho)$ with cylinder symmetry. As in crystal channeling, the averaging over z is well justified as a collision of a particle with a nanotube wall under a glancing angle does involve many thousand atoms along the particle trajectory. For the same reason, the averaging over ϕ is equally justified if the nanotube has an arbitrary helicity [22] as defined by nanotube indices (m, n). In the special cases of zigzag (m = 0) or armchair (m = n)nanotubes, the wall consists of atomic rows parallel to the nanotube axis; the nanotube potential is then defined by the sum of potentials of the rows, and this case deserves a separate consideration. Further on in the Letter we apply only the averaged potential $U(\rho)$ for a straight nanotube. This approach reveals the general features of nanotube channeling.

In a carbon SWNT, the channeled particles are confined in a potential well $U(\rho)$ with the depth U_0 of about 60 eV. The field experienced by a high-energy particle moving in an aligned MWNT is the sum of the fields of single walls of different diameter with the same axis. In addition to atomic potentials, in a nanotube bent with radius *R*, an effective potential taking into account a centrifugal term pvx/R is introduced similarly to bent crystals [1]:

$$U_{\text{eff}}(\rho, \phi) = U(\rho, \phi) + \frac{pvx}{R}$$

where $x = r \cos(\phi)$ is the coordinate in the direction of bending, pv is the particle momentum times velocity.

We use so-called standard potential introduced by Lindhard [25]. When averaged over (ϕ, z) , the potential of SWNT is described by [17]:

$$U_{\text{SWNT}}(\rho) = \frac{4NZ_1Z_2e^2}{3a} \times \ln\left(\frac{r^2 + \rho^2 + 3a_S^2}{|r^2 - \rho^2| + r^2 + \rho^2} + \frac{\sqrt{(r^2 + \rho^2 + 3a_S^2)^2 - 4r^2\rho^2}}{|r^2 - \rho^2| + r^2 + \rho^2}\right).$$

Here Z_1e , Z_2e are the charges of the incident particle and the nanotube nuclei, respectively, N is the number of elementary periods along the tube perimeter, a =0.142 nm is the carbon bond length; the SWNT radius is $r = Na\sqrt{3}/2\pi$.

The screening distance a_S is related to the Bohr radius a_B by

$$a_{S} = \frac{a_{B}}{2} \left(\frac{3\pi}{4(Z_{1}^{1/2} + Z_{2}^{1/2})} \right)^{2/3} \tag{1}$$

for interaction between neutral atoms. In the Gemmel's review [26] this formula is applied also to partially ionized projectiles. Further discussion of screening distance can be found in Ref. [26]. For a point-like charge or fully ionized projectile, a simpler formula is used:

$$a_S = \frac{a_B}{2} \left(\frac{3\pi}{4}\right)^{2/3} Z_2^{-1/3}.$$
 (2)

The potential $U(\rho)$ of MWNT is the sum of contributions of SWNT making up the MWNT. Actually, only the two adjacent walls contribute sizably for the particle located between them.

In a tube bent along the *x* direction, the motion of a particle is described by the equations

$$pv\frac{d^{2}x}{dz^{2}} + \frac{dU(\rho)}{dx} + \frac{pv}{R(z)} = 0,$$
(3)

$$pv\frac{d^2y}{dz^2} + \frac{dU(\rho)}{dy} = 0,$$
(4)

where $\rho^2 = x^2 + y^2$. This takes into account only the nanotube potential and the centrifugal potential. Any particle within close distance, order of a_S , from the wall (where density of the nuclei is significant) is also strongly affected by the nuclear scattering.

Two mechanisms of particle transfer from channeled to random states are well known for crystals: scattering on electrons and nuclei and curvature of the channel [1]. A typical nanotube is less than 0.1 mm in length at present. For such a short channel, the scattering on electrons within the bulk of the tube is insignificant for high-energy particles. However, a curvature of the tube could quickly (in less than one oscillation) bring much of the channeled particles out of the potential well or into close collisions with the nuclei of the nanotube walls.

Fig. 1(a) shows an example of the trajectory of a particle channeled in a straight MWNT, trapped between the pair of adjacent walls. The radial motion of the channeled particle is finite while in azimuthal direction it is free. Fig. 1(b) shows an example of the trajectory when MWNT is weakly bent; obviously, the particle is localized in some range of ϕ to conform to a centrifugal force when moving along a bent nanostructure. An example of the stronger bending is illustrated by Fig. 1(c).

As a result of bending, the MWNT phase-space of transverse coordinates and transverse angles available for channeled particles is reduced. The particles channeled through a bent MWNT are deflected at the angle of MWNT bending. Fig. 2 shows an example of the angular distribution of particles downstream of the 50- μ m long MWNT bent 5 mrad, shown in the direction of bending. Similarly to the pictures of bent crystal channeling, there is clear separation of channeled and nonchanneled peaks, with some particles lost (dechanneled along the tube) between the peaks.

This example shows that channeled particles can survive in a bent MWNT, so the effect could be used for steering of high-energy particles provided its efficiency in MWNT is good enough compared to SWNT and crystal lattices.

3. Comparison of MWNT to SWNT and to crystal lattice

While the capability of MWNT to channel particles could be hoped for from the standpoint of channeling



Fig. 1. An example of the trajectory of a 1-GeV proton injected between two walls of a straight MWNT (a); the same in a slightly bent (b), R = 14 cm, and strongly bent (c), R = 3 cm, MWNT.

theory, just from the existence of channels, the channeling efficiency of MWNT relative to other channeling structures such as SWNT and crystal lattices is not obvious at all, unless this issue is studied in Monte Carlo simulations. We looked in simulations how channeled particles survive in multi-wall nanotubes of different curvatures. The Monte Carlo studies of nanotube channeling efficiency were done over a broad range of bendings for the nanotube, and with a range of MWNT size (in-

particle distribution downstream of bent MWNT



Fig. 2. An example of 1-GeV proton angular distribution downstream of a bent MWNT, in the direction of bending.

ner and outer diameters) about its typical value in a synthesized MWNT. A parallel beam of 1 GeV protons was entering a carbon nanotube, where protons were tracked over 50 μ m. Multiple scattering was not included, so we did evaluate only the effects of bending dechanneling. Fig. 3 shows the number of protons channeled through 50 μ m of MWNT as a function of the centrifugal force pv/R; for comparison, we also show the same function for SWNT and Si(110) crystal lattice.

Fig. 3 shows similar slopes of the curves for MWNT, SWNT and Si(110), this means that the number of channeled particles in a MWNT declines at a rate similar to that in the other efficient channeling structures. This holds true both for the moderate bendings from 0.1 to 1 GeV/cm (equivalent to 30-300 T magnetic field, Fig. 3(a)) where silicon channeling crystals are used for beam steering at the high-energy accelerators nowadays, and for the strong bendings of 1-4 GeV/cm (equivalent to 300-1200 T, Fig. 3(b)). Such a study was done for MWNT of different external and internal diameter, and the same results were obtained; the parameter that matters was the interwall spacing fixed at 0.34 nm. Notice that MWNT competes with the best of SWNT (≤ 1 nm diameter) while wider SWNT (≥ 1 nm) are less efficient in steering (bending) of the channeled particles.



Fig. 3. The number of 1-GeV protons channeled through a bent MWNT (50 μ m long) shown as a function of the centrifugal force pv/R; for comparison, also shown is the same dependence for SWNT (diameters 0.55 nm and 11 nm) and for Si(110) crystal lattice. Two ranges were studied: moderate bendings (a) and strong bendings (b).

4. Further research and potential applications

The feasibility of experiments to test channeling and coherent scattering with the existing samples of very short (tens of micron) nanotubes at high energy accelerators has been demonstrated in Monte Carlo simulations [27,28]. These studies could be extended also to the comparison of MWNT versus SWNT. Such experiments are in preparation at IHEP and LNF. Practical considerations, such as the demand for a good alignment within the array of nanotubes, could play a leading role in the choice of nanostructured material for channeling studies. Since we have shown that MWNT are at least as good channeling structures as SWNT, further considerations driven by technology

channeled particles

may well switch the general interest from SWNT to MWNT as channeling candidates. While SWNT are very curly on production in general, MWNT are quite straight and come in aligned arrays, which is a great technological advantage in view of channeling application.

With high energy beams and typically short nanotubes available, the issue of *dechanneling length* due to scattering on electrons within the bulk of the tube is less important at the time. However, this issue is physically very interesting because of low electronic density (and hence low electronic scattering) in the bulk of the nanotube, and it deserves a special study.

Whereas the interest to nanotube channeling at this early stage is more academic, some application can be quoted in relation with unique capabilities of nanotube channeling. There is a need in beams of very small emittance, "microbeams" or even "nanobeams", and channeling technique can be a help here [13]. The capability to produce beams with very small crosssection, i.e., "nano-beams", will be helpful in medical, biological, and technological applications. We refer to [13,29] for discussion of it.

5. Summary

Channeling and centrifugal dechanneling phenomena have been demonstrated and studied for positively charged particles in MWNT. As shown in computer simulations, MWNT can channel particle beams with efficiency similar to that of crystal channeling, and to that of SWNT, despite the fact that the geometry of MWNT, and respectively the potential wells where channeled particles can be trapped, are very different from the case of SWNT.

Together with the advantage of MWNT produced typically quite straight (unlike SWNT with strong parasitic curvature) and in aligned arrays, this finding suggests that a MWNT is a better candidate for channeling than a SWNT. Multi-wall nanotubes could make a basis for an efficient technique of beam steering at particle accelerators.

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