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CHANNELING POTENTIAL THROUGH RADIAL DEFORMED TRIPLE WALL CARBON NANOTUBES

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Abstract. In this study we presented a theoretical investigation of the channeling interaction potential between proton and the radial deformed (12, 0)@(8, 0)@(4, 0) triple-wall carbon nanotubes (TWNTs). Multi-wall nanotubes (MWNTs) can be technically realised with better channeling performance than the single-wall nanotubes (SWNTs) and that is why we believe that these investigations can be useful for guiding of nanosized ion beams. Obtained results show that the channeling potential is strongly influenced of level of radial deformation of nanotube.

1. INTRODUCTION

After the discovery of the carbon nanotubes, a lot of theoretical groups started to work on theoretical modeling and computer simulation of ion channeling through carbon nanotubes, see Artru et al. 2005 and Borka et al. 2011 and references therein. The experimental advancement in this area is still in the very beginning (Zhu et al. 2005, Chai et al. 2007). The both mentioned experiments are performed with the well aligned MWNTs, and that is why we study MWNTs in this paper.

Carbon nanotube can be radially deformed if we apply external mechanical stress (Hasegawa & Nishidate 2006, Imtani & Jindal 2007) or external electric field (Shtogun & Woods 2009, Kan et al. 2010) or if we use atomic force microscope (Shtogun & Woods 2009). The presence of deformations influence strongly on the nanotube's channeling properties (Abu-Assy & Soliman 2016). This work is continuation of our previous investigation (Borka Jovanović et al. 2017, Borka & Borka Jovanović 2019, Borka & Galijaš 2019). In this work we have presented a theoretical investigation of the channeling potential with the radial deformed TWNTs(12, 0)@(8, 0)@(4, 0).

2. THEORY

In this work we assumed the continuum model approximation (Lindhard 1965, Gemmel 1974). We calculate the proton nanotube interaction potential $U(x, y)$ as a function of the proton-atom distance r. We used the Molière's approximation of

the Thomas-Fermi interaction potential (Molière 1947) $V(r)$ in the following form: $U(x,y) = \sum_{k=1}^{J} \frac{1}{d} \int_{-\infty}^{\infty} V\left(\sqrt{\rho_k^2 + z^2}\right) dz$, 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 centres 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 nanotube is indicated by J and in our case it is 48 (see Figure 1).

3. RESULTS AND DISCUSSION

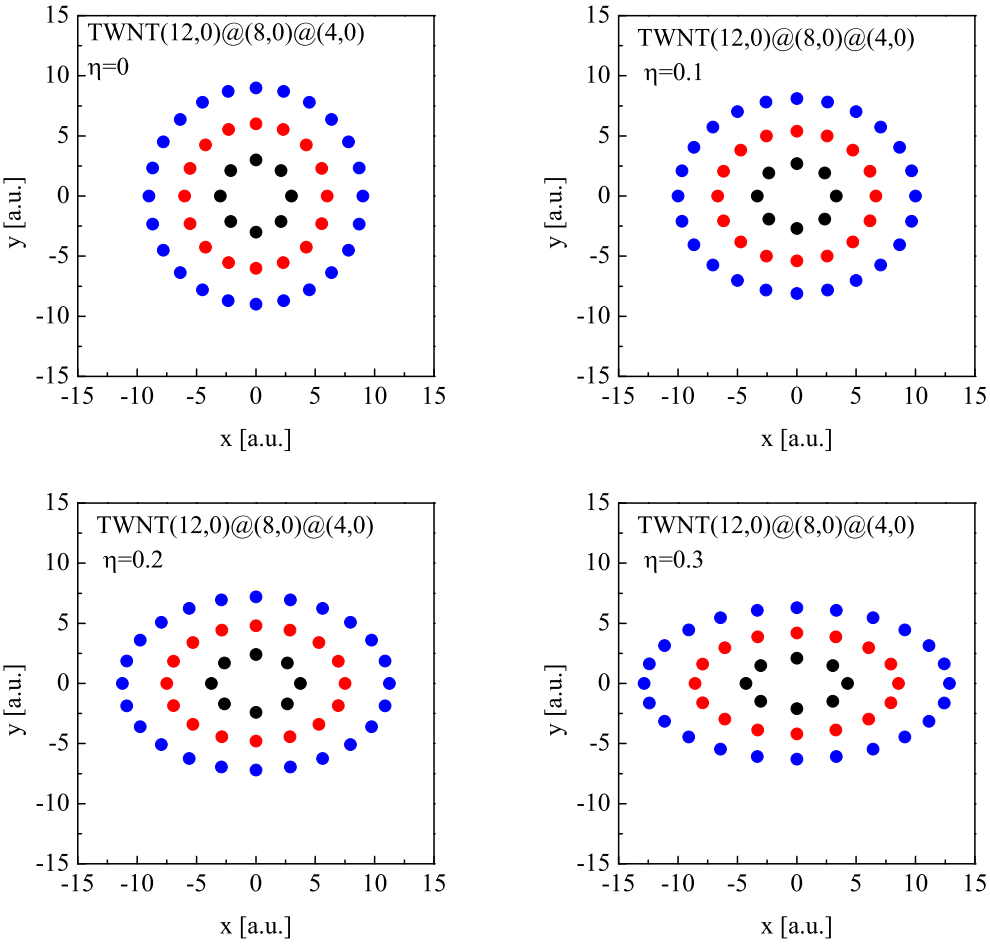

Figure 1: The view along axes of short TWNTs(12, 0)@(8, 0)@(4, 0) under different radial strains: (left top) $\eta = 0$ (perfect nanotube); (right top) $\eta = 0.1$; (left down) $\eta = 0.2$; (right down) $\eta = 0.3$, respectively.

Here, we have analyzed from theoretical aspect the channeling interaction poten-

tial of protons and the radial deformed TWNT(12, 0)@(8, 0)@(4, 0). We take into account the effect of the radial deformation because majority of nanotubes are radially deformed. Radial deformation is characterized by the dimensionless parameter $\eta = (R - R_y)/R$, where R_y is semi-minor axis and R is the radius of underfomed nanotube (Shtogun & Woods 2009). Also, we can express the semi-axis as a function of the radius R and the parameter η: $R_x = R(1-\eta)^{-1}$ and $R_y = R(1-\eta)$.

We study 4 different cases of short TWNT(12, 0)@(8, 0)@(4, 0): for perfect nanotube ($\eta = 0$) and under three different radial strains: $\eta = 0.1$, 0.2 and 0.3. From Figure 1 we can see that the intersection of the nanotube with the transverse plane gives an ellipse with semi-major axis R_x and semi-minor axis R_y. We can conclude that the radial cross section of the nanotube can take different elliptical shapes depending on the values of parameter η.

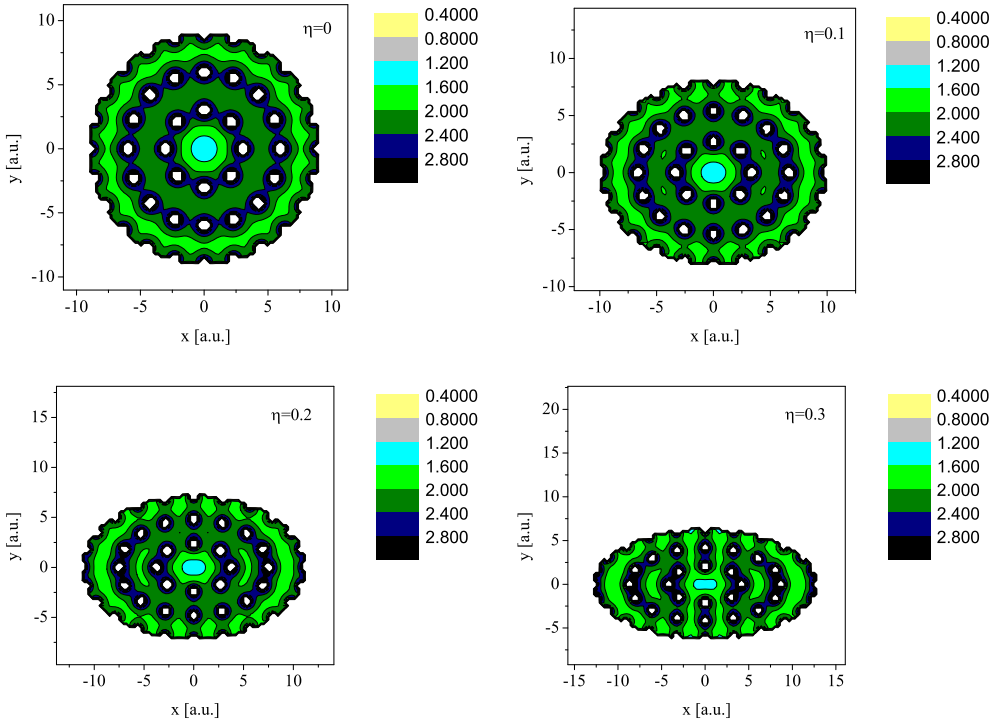

Figure 2: Contour plot of the channeling interaction potential $U(x, y)$ in the xy plane between proton and TWNTs(12, 0)@(8, 0)@(4, 0) under different radial strains: (left top) $\eta = 0$; (right top) $\eta = 0.1$; (left down) $\eta = 0.2$; (right down) $\eta = 0.3$, respectively. Values for potential U(x,y) within nanotube are presented in atomic units.

The radius of carbon nanotube R is: $R = l\sqrt{3}(2\pi)^{-1}\left(n^2 + nm + m^2\right)^{1/2}$, where the (n, m) represents chiral index and l represents interatomic length (the bond length between carbon atoms ≈ 0.144 nm (Saito et al. 2001)). 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: $\theta_k = \arctan\left(\frac{R_y}{R_x}\tan\left(2\pi(k-1)/N\right)\right)$, rel-

ative to the semi-major axis and the distance from the nanotube center: $R_k = \left(R_x^{-2} - \sin^2\theta_k \left(R_x^{-2} - R_y^{-2}\right)\right)^{-1/2}$.

The interaction potential can be calculated using following equation: $U(x,y) = \frac{4Z_1Z_2e^2}{d} \times \sum_{k=1}^{N} \sum_{j=1}^{3} a_j K_0 \left(b_j \sqrt{x^2+y^2+R_k^2 - 2\sqrt{x^2+y^2}R_k\cos\theta_k}\right)$, where $Z_1 = 1$ and $Z_2 = 6$ are the atomic numbers of the proton and carbon atom, respectively, e is the elementary charge, $a_1 = 0.35$, $a_2 = 0.55$, $a_3 = 0.1$, $b_1 = 0.3/a_{tf}$, $b_2 = 1.2/a_{tf}$, $b_3 = 6/a_{tf}$, where $a_{tf} = (9\pi^2/(128Z_2))^{1/3}a_0$ is the screening Thomas-Fermi radius, and a_0 is Bohr radius.

We can notice that the TWNT(12, 0)@(8, 0)@(4, 0) consists of SWNT(12, 0), SWNT(8, 0) and SWNT(4, 0). We can calculate the total interaction potential like: $U(x,y)_{TWNT} = U(x,y)_{SWNT(12,\ 0)} + U(x,y)_{SWNT(8,\ 0)} + U(x,y)_{SWNT(4,\ 0)}$.

Figure 2 shows contour plots of the channeling interaction potential $U(x,y)$ in the xy plane of proton and TWNT(12, 0)@(8, 0)@(4, 0) for perfect straight nanotube ($\eta = 0$) and for nanotubes under three different radial strains. Values for potential U(x,y) within nanotubes are presented in atomic units. The potential is changing very quickly close to atomic rows and the changing of potential is very slowly near the nanotube center where is the minimum value of potential. We can conclude that the nanotube channeling potential depends strongly on the radial strain.

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References

Abu-Assy, M. K. & Soliman, M. S.: 2016, *Nucl. Instrum. Meth. Phys. Res. B* **384**, 93.
Artru, X. et al.: 2005, *Phys. Rep.* **412**, 89.
Borka, D., Petrović, S., Nešković, N.: *Channeling of protons through carbon nanotubes*, Nova Science Publishers, ISBN 978-1-61122-050-6, New York (2011).
Borka Jovanović, V., Borka, D., Galijaš, S. M. D.: 2017, *Phys. Lett. A* **381**, 1687.
Borka, D. & Borka Jovanović, V.: 2019, *Atoms* **7**, 88.
Borka, D. & Galijaš, S. M. D.: 2019, *Rom. Rep. Phys.* **71**, 207.
Chai, G., Heinrich, H., Chow, L., Schenkel, T.: 2007, *Appl. Phys. Lett.* **91**, 103101.
Gemmell, D. S.: 1974, *Rev. Mod. Phys.* **46**, 129.
Hasegawa, M. & Nishidate, K.: 2006, *Phys. Rev. B* **74**, 115401.
Imtani, A. N. & Jindal, V. K.: 2007, *Phys. Rev. B* **76**, 195447.
Kan, B. et al.: 2010, *Nanoscale Res. Lett.* **5**, 1144.
Lindhard, J. K.: 1965, *Dan. Vidensk. Selsk., Mat.-Fys.Medd.* **34, No. 14**, 1.
Molière, G.: 1947, *Z. Naturforsch. A* **2**, 133.
Saito, R., Dresselhaus, G., Dresselhaus, M. S.: *Physical Properties of Carbon Nanotubes*, Imperial College Press, London (2001).
Shtogun, Y. V. & Woods, L. M.: 2009, *J. Phys. Chem. C* **113**, 4792.
Zhu, Z. et al.: 2005, *Proc. of the Int. Conf. on Charged and Neutral Particles Channeling Phenomena*, **5974** (Bellingham, Washington: SPIE) pp 1-13.