CHANNELING POTENTIAL THROUGH RADIAL DEFORMED TRIPLE WALL CARBON NANOTUBES

DUŠKO BORKA and VESNA BORKA JOVANOVIĆ

Department of Theoretical Physics and Condensed Matter Physics (020), Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

e-mail: dusborka@vinca.rs, vborka@vinca.rs

VINČA INSTITUTE OF NUCLEAR SCIENCES

➢ 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 [1]. Obtained results show that the channeling potential is strongly influenced of level of radial deformation of nanotube [2, 3, 4].

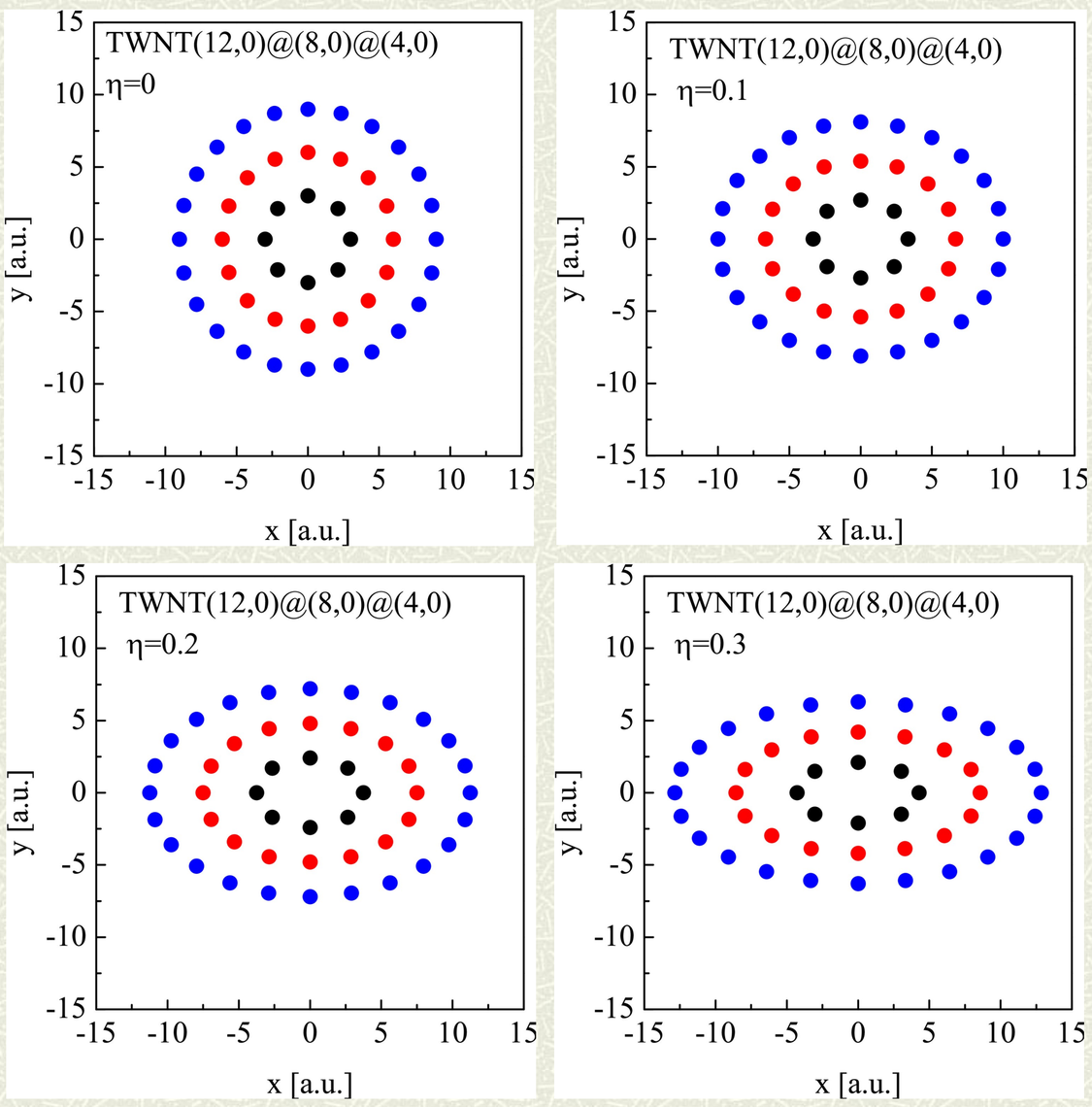

Figure 1. The view along axes of short TWNTs(12,0)@(8,0)@(4,0) under different radial strains: (left top) η = 0 (perfect nanotube); (right top) η = 0.1; (left down) η = 0.2; (right down) η = 0.3, respectively.

➢ We take that the interaction potential of the proton and a nanotube atom is of the Thomas-Fermi type and adopt for it the Molière's expression [5, 6, 7]:

$$V(r') = \frac{Z_1 Z_2 e^2}{r'}\left(0.35e^{-0.3r'/a} + 0.55e^{-1.2r'/a} + 0.10e^{-6.0r'/a}\right)$$

Z_1 = 1 and Z_2 = 6 are the atomic numbers of the proton and nanotubes atoms, respectively

r – the distance between the proton and the nanotube atoms, b = 0.3/a – parameter

$a = [9\pi^2/(128\ Z_2)]^{1/3}a_0$ – the screening radius of the atom

a_0 – the Bohr radius (52.918 pm).

When we apply continuum approximation [6, 8] as a result, we obtain the proton- nanotube continuum interaction potential:

$$U(x,y) = \sum_{j=1}^{J} U_j(x,y); \quad U_j(x,y) = \frac{1}{d}\int_{-\infty}^{+\infty} V\left(\rho_j^2 + z^2\right)^{1/2} dz$$

$$\rho_j = \left((x - x_j)^2 + (y - y_j)^2\right)^{1/2}$$

➢ The total number of atomic strings in the nanotube is indicated by J and in our case it is 48 (see Figure 1).

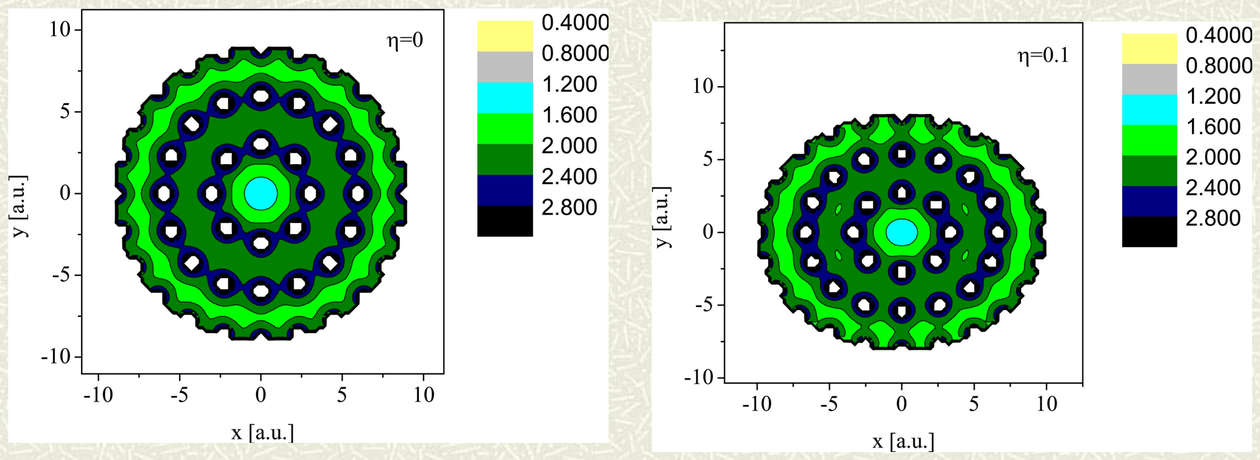

Figure 2. Contour plot of the channeling interaction potential U (x, y) in the xy plane between proton and TWNTs(12,0)@(8,0)@(4,0) under different radial strains: (left top) η = 0; (right top) η = 0.1; (left down) η = 0.2; (right down) η = 0.3, respectively. Values for potential U(x,y) within nanotube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

Radial deformation is characterized by the dimensionless parameter $\eta = (R - R_y)/R$ [9, 10, 11], where R_y is semi-minor axis and R is the radius of undeformed nanotube. 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 $R_y = R(1 - \eta)$.

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 θ_k and the distance from the nanotube center is R_k.

The interaction potential U(x,y) can be calculated using following equation:

$$U(x,y) = \frac{4Z_1 Z_2 e^2}{d} \times \sum_{k=1}^{N}\sum_{j=1}^{3} a_j K_0\left(b_j\sqrt{x^2 + y^2 + R_k^2 - 2\sqrt{x^2 + y^2}R_k\cos\theta_k}\right.$$

We can conclude that the nanotube channeling potential depends strongly on the radial strain.

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