Energy Spectrum of Relativistic Positrons Channeled Through Single-wall Carbon Nanotubes

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We calculate the energy eigenvalues of the channeled positrons through single wall carbon nanotubes (n,m). According to the continuum model approximation given by Lindhard for the case of an axial channeling in single crystals, the actual periodic potential of a row of atoms is replaced by a potential averaged over a direction parallel to the row, called continuum potential. The calculations was executed by using the atomic interaction potential as given by Moliere potential and Biersack's universal potential. The maximum number of bound states and the energy eigenvalues is calculated for positrons of 100 MeV energy incident in a direction parallel to the nanotube axis, by using WKB method. The calculations showed that the estimation of the maximum number of bound states of the channeled positron in armchair, chiral, and zigzag nanotubes is higher for the Moliere potential than for the Universal potential. The calculations showed that the effect of temperature by using Debye approximation of thermal vibration amplitude on the channeling potential is very small and gave the same eigenvalues and the same number of bound states as that for the static nanotubes.

1. Introduction

A great variety of physical processes can occur when an energetic beam of charged particles is incident upon a solid target. All of these processes have cross sections, which depend on the impact parameters involved in collisions with individual target atoms. If the target material is monocrystalline, the distribution of the impact parameters and the yield of physical processes was found to be very strongly dependent on the relative orientation of the beam direction and the target. This effect is called the "channeling" effect. Much of the basic theory of the channeling process can be found in the treatment published by Lndhard in 1965 [1]. Channeling effect has found several important applications [2]. In our previous work, special consideration is devoted to the channeling of positively charged particles in disordered lattices of cubic crystals including the characteristics of channeling radiation that emits spontaneously due to transitions between eigenstates of the channeled positrons [3] in addition to calculations of the transmission and dechanneling coefficients in disordered lattices, [4-7].

The channeling effect in single-wall carbon nanotubes SWCNT's has found many important advantages compared to single crystals [8, 9], for example:

- SWCNT's have much wider channels than ordinary crystals, implying weaker dechanneling so that, longer channeling distances may be achieved.
- The wider channeling angle in SWCNT's (up to (~ 0.1 rad) are accepted for ion channeling in SWCNT's than in ordinary crystals, leads to the possibility of ion channeling at low energies (~ 1 KeV), which recently found great interest in the field of molecular dynamic simulations.
- The channeling potential wells of nanotubes are sufficiently deep and broad to allow an efficient capture of positive particle beam in channeling states. Moreover , for nanotube ropes, the low electron and atomic density inside the channel make their channeling more stable than in ordinary crystals.

In addition to several possible uses of Ion channeling through carbon nanotube as a diagnostic tool analyzing the structure of nanotubes, there is a wide range of potential applications of the channeling through SWCNT's in other areas, for example [8,9]:

- Creation and transportation of highly focused nano-beams.
- Ion implantation in manufacturing nano-elecronics devices.
- Extraction, steering and collimation of ion beams at high energy particle accelerators.

A SWCNT's can be thought of as resulting from rolling a strip of graphene into a cylinder. Graphene is a single planar sheet of sp^2- bonded carbon atoms forming a hexagonal lattice with the bond length of $\ell \approx 0.141\,\text{nm}$ between carbon atoms, giving the surface density of atoms $\sigma_{at} = 4/(3^{3/2}\ell)$. A roll-up vector, which generates the circumference of a SWCNT, can be defined in the graphene strip by $\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2$, where $\mathbf{a}_1$ and $\mathbf{a}_2$ are the basis vectors (with the angle $\pi/3$ between them and $|\mathbf{a}_1| = |\mathbf{a}_2| = \ell\sqrt{3}$), forming a rhomboidal unit cell of graphene [10]. The pair of integers (n,m) completely determines the atomic structure of any SWCNT and specifically, its diameter, $d = (\ell\sqrt{3}/\pi)\sqrt{n^2 + nm + m^2}$, helicity or chiral angle $\theta = \arctan[\sqrt{3}m/(m+2n)]$, as well as its longitudinal periodicity. SWCNT's with $m = 0 (\theta = 0^o)$ are called *zigzag*, those with $m = n (\theta = 30^o)$ *armchair*, while all other with $0 < m < n$ are called *chiral* nanotubes.

The system under investigation is a channeling of relativistic positrons through an (n,m) single-wall carbon nanotube (SWCNT). The nanotube axis is in z-direction and the origin lies at the transverse entrance plane. The motion of positrons in this channeling regime is governed by a transverse potential and we can find the bound states and the maximum number of bound states for the given incident energy. The initial positron velocity taken to be parallel to z-axis. We assume that the nanotube is sufficiently short for the positron energy loss to be neglected.

In this work we consider the channeling of 100 MeV positrons through single-wall carbon nanotubes (10,10) , (11,9) and (18,0).

2. Channeling Potential in Carbon Nanotubes

According to the continuum model approximation given by Lindhard [1] for the case of an axial channeling in single crystals, the actual periodic potential of a row of atoms is replaced by a potential averaged over a direction parallel to the row, called continuum potential. The continuum potential of single atomic row can be written as:

$$V(r) = \frac{1}{d_R}\int_{-\infty}^{\infty} V(\sqrt{r^2+z^2})dz \tag{1}$$

where V is the atomic interaction potential, r is the distance from the row, z is the coordinate along the row and d_R is the average distance of neighboring atoms along the row. If a fast charged particle enters a nanotube at small angle to the tube axis (i.e., in channeling regime), the motion of the particle is governed by a continuum potential as given by Eq. (1).

In this work, the calculations is executed by using the atomic interaction potential as given by Moliere potential [11] and Biersack's universal potential [12] respectively as:

$$V_M(\mathbf{x}) = \frac{z_1 z_2 e^2}{x}\sum_{i=1}^{3}\alpha_i \exp(-\beta_i \mathbf{x}) \tag{2}$$

with $\{\alpha_i\} = \{0.35, 0.55, 0.1\}, \{\beta_i\} = \{0.3/a, 1.2/a, 6/a\}$ where $a = (9\pi^2/128z_2)^{1/3}a_0$, is the Thomas-Fermi screening radius; $a_0 = 0.529\,\text{Å}$ is the Bohr radius, z_1 and z_2 are the charge numbers of projectile and target atoms, respectively, e is the elementary charge and x is the separation between them.

$$V_U(\mathbf{x}) = \frac{z_1 z_2 e^2}{x}\sum_{i=1}^{4} p_i \exp(-q_i \mathbf{x}) \tag{3}$$

with $\{p_i\} = \{0.18175, 0.50986, 0.28022, 0.02817\}$,

$\{q_i\} = \{3.1998/a, 0.94229/a, 0.40296/a, 0.20162/a\}$

Using the above expressions given by Eq. (2) and Eq. (3) in Eq. (1), we can obtain the axial potential corresponding to Moliere and Biersack's universal potentials respectively as:

$$U_M(r) = \frac{2z_1 z_2 e^2}{d_R}\sum_{i=1}^{3}\alpha_i K_0(\beta_i r), \tag{4}$$

$$U_U(r) = \frac{2z_1 z_2 e^2}{d_R} \sum_{i=1}^{4} p_i K_0(q_i r), \tag{5}$$

where K_0 is the modified Bessel function of the second kind and order zero.

The channeling potential of a nanotube $U(\boldsymbol{\rho})$, where $\boldsymbol{\rho}$ is a vector normal to the tube axis, is the sum of the axial potentials given by Eq. (4) or Eq. (5) of the rows positioned at $\mathbf{r}_i$ over the circumference of the nanotube (Fig. 1), i.e.,

$$U(\boldsymbol{\rho}) = \sum_{i=1}^{N} U(|\boldsymbol{\rho} - \mathbf{r}_i|) \tag{6}$$

where $N = (2/q)(n^2 + nm + m^2)$ is the number of atomic rows [8], with, $q = \gcd(2m+n, 2n+m)$ denotes the greatest common divisor of its arguments. In the numerical calculation of Eq. (6), we note that, the N rows consists of two sequences of rows overlap with a doubled linear atomic density $2/d_R$.

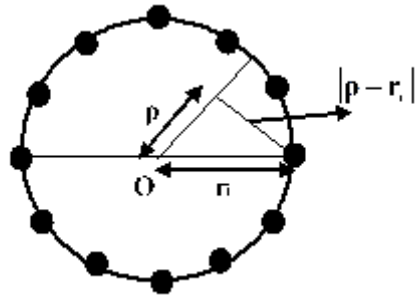

Fig. (1): Cross section of the nanotube channel is a circle of radius r, the rows of the carbon atoms are positioned at $\mathbf{r}_i$ over the circumference of the nanotube, $\boldsymbol{\rho}$ the distance from the nanotube center.

The effect of thermal vibrations on channeling potential in carbon nanotube can be estimated by modification in the axial potential. In this work an expression for the axial potential at large distance from the nanotube wall was used which based on the Moliere atomic interaction due to one raw modified by the effect of thermal vibration is given by [13]:

$$U_{MT}(r) = \frac{2z_1 z_2 e^2}{d_R} \sum_{i=1}^{3} \alpha_i K_0(-\beta_i r) e^{(u_1^2/2\alpha_i^2)}, \tag{7}$$

where u_1 is the thermal vibrational amplitude of the carbon atoms estimated from the Debye approximation [2], as shown in Fig. (2).

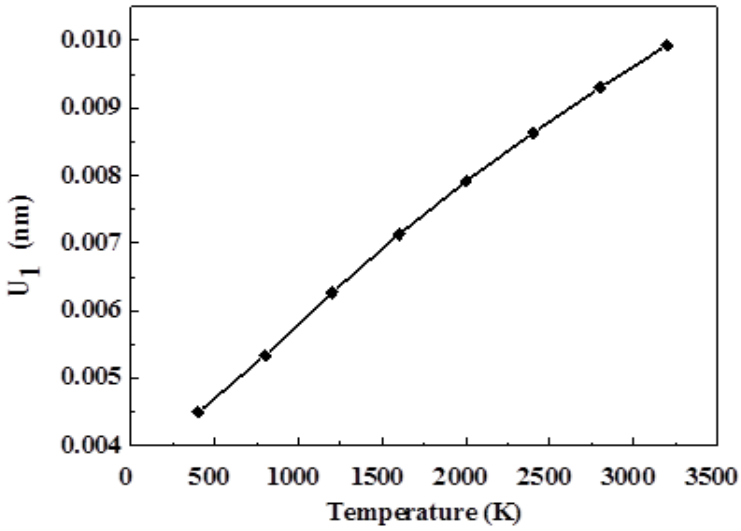

Fig.(2): Thermal vibration amplitude u_1 for carbon atoms as a function of temperature using the Debye approximation [2].

3. Calculation of the Energy Eigenvalues

We find that an expression of the form

$$U(\rho) = a_1 + b_1 e^{c_1 \rho} \tag{8}$$

is a reasonable approximation for the channeling potential calculated in Ref. [14] and in this work by using Moliere and Biersack's universal potentials using Eqs. (4), (5) and (6). The parameters a_1, b_1 and c_1 are given in Table 1 for carbon nanotubes under consideration and ρ is measured from the center of the tube in a plane normal to the tube axis.

We use the WKB method [15], to obtain the energy eigenvalues of the channeled positrons constrained to move between classical turning points ρ_1 and ρ_2 in a potential given by Eq. (8). The classical turning points are those points at which $U(\rho) = E$ that is

$$E = a_1 + b_1 e^{c_1 \rho} \quad \text{or} \quad \rho_1 = -(1/c_1)\ln[(E - a_1)/b_1]$$

and

$$\rho_2 = (1/c_1)\ln[(E - a_1)/b_1]$$

For a particle constrained to move between classical turning points ρ_1 and ρ_2 in a potential well the energy eigenvalues can be obtained from the condition [15].

$$\int_{\rho_1}^{\rho_2} p\, d\rho = (n + \frac{1}{2})\pi\hbar \,, \qquad n = 0, 1, 2, ... \tag{9}$$

where $p = \left[2m_0\gamma\left(E - \left(a_1 + b_1 e^{c_1\rho}\right)\right)\right]^{1/2}$, is the classical linear momentum, m_0 is the positron rest mass and γ is the relativistic correction. Then, from Eq. (9), we can get the energy eigenvalues and the maximum number of bound states respectively as:

$$E_n = a_1 + \left(\frac{1}{2m_0\gamma}\right)\left(\frac{c_1\pi\hbar}{2\ln 2}\right)^2 (n+\frac{1}{2})^2 \tag{10}$$

and

$$n_{\max} = \left(\frac{2\ln 2}{c_1\pi\hbar}\right)\left[2m_0\gamma(E_{\max} - a_1)\right]^{1/2} - 0.5 \tag{11}$$

where E_{max}, is the potential at the turning points, that is $E_{\max} = a_1 + b_1 e^{c_1 s}$, $s = R - a$, is the screening length with $R = d/2$ being the nanotube radius.

3. Computational Results and Discussion

Thermal vibrational amplitude u_1 for carbon atoms as a function of temperature using the Debye approximation [2] is shown in Fig. (2).

Channeling potential $U_{th}(\rho)$ of positrons channeled in (11,9) single wall carbon nanotube at thermal vibration amplitude u_1 = 0.0053 *nm* (i.,e., at ~ 790 K) by using Debye approximation as a function of a distance ρ from the center of the tube in a plane normal to the tube axis is shown in Fig. (3). The curve represents the present work by using Moliere atomic potential with the effect of thermal vibration Eq. (7) and the channeling potential as given in Ref. [14]. The two models gave the same numerical result.

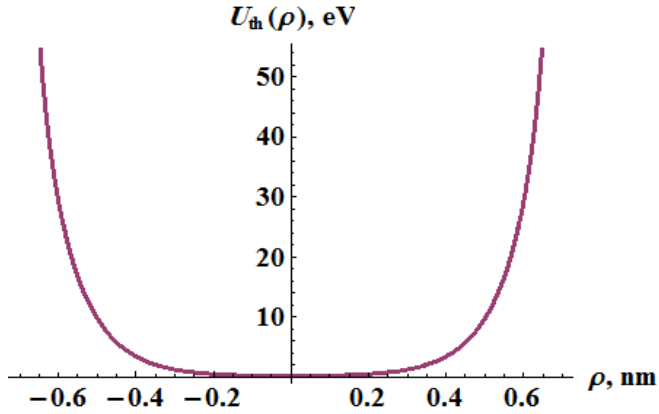

Fig. (3): Channeling potential of positrons channeled in (11,9) single wall carbon nanotube as a function of a distance ρ from the center of the tube in a plane normal to the tube axis. The curve represents the present work by using Moliere atomic potential and the potential as given in Ref. [14]. The calculations is executed at thermal vibration amplitude $u_1 = 0.0053\,\text{nm}$.

The numerical results showed that the effect of thermal vibrational amplitude on the channeling potential is very small and gave the same results as that for the channeling potential of static nanotube for all possible values of thermal vibrations.

The calculations of the channeling potential $U(\rho)$ as given by Eq. (6), in single wall carbon nanotube for positrons channeled in armchair, chiral, and zigzag nanotubes is illustrated by the solid curve for (10,10), (11,9) and (18,0) in Figs. (4, 5, and 6), respectively by using Moliere and Biersack's universal potentials. The bound states, as given by Eq. (10), corresponding to channeling of 100 MeV positrons incident in the direction parallel to the nanotube axis is also shown in each figure and is illustrated by the horizontal lines.

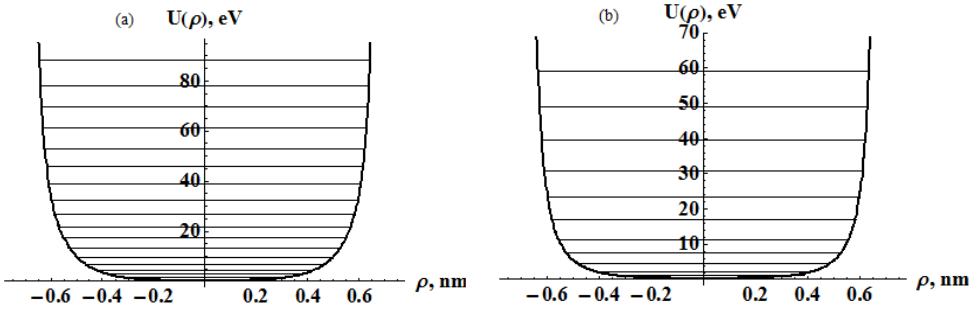

Fig. (4): Channeling potential of positrons channeled in an (10,10) single wall carbon nanotube as a function of a distance ρ from the center of the tube in a plane normal to the tube axis, (a) Moliere atomic potential, (b) Universal atomic potential. Some eigenvalues of 100 MeV positrons incident in the direction parallel to the nanotube axis are shown by horizontal lines.

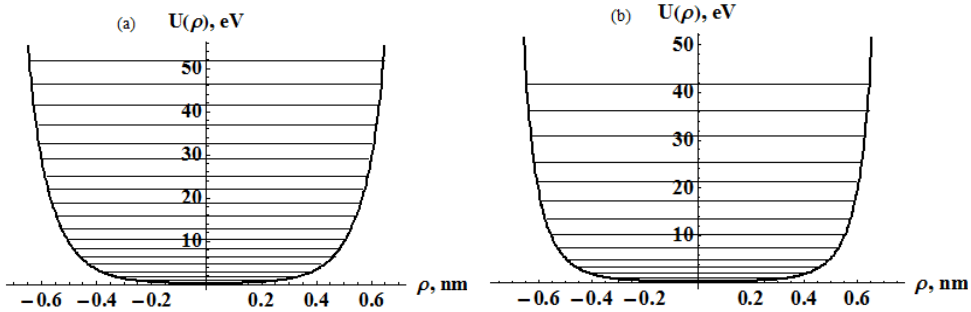

Fig. (5): Channeling potential of positrons channeled in an (11,9) single wall carbon nanotube as a function of a distance ρ from the center of the tube in a plane normal to the tube axis, (a) Moliere atomic potential, (b) Universal atomic potential. Some eigenvalues of 100 MeV positrons incident in the direction parallel to the nanotube axis are shown by horizontal lines.

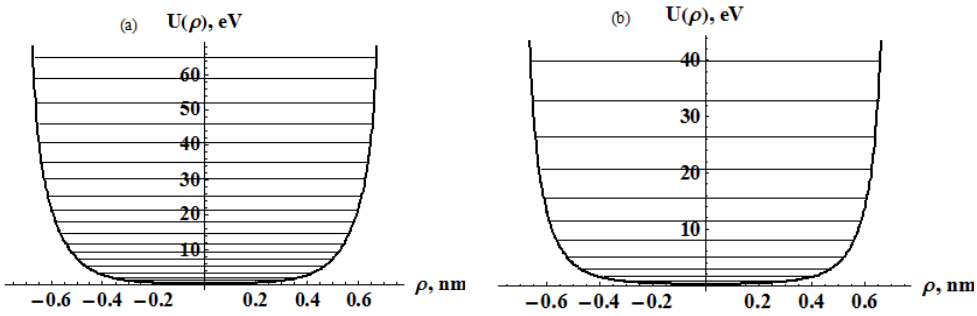

Fig. (6): Channeling potential of positrons channeled in an (18,0) single wall carbon nanotube as a function of a distance ρ from the center of the tube in a plane normal to the tube axis, (a) Moliere atomic potential, (b) Universal atomic potential. Some eigenvalues of 100 MeV positrons incident in the direction parallel to the nanotube axis are shown by horizontal lines.

The maximum number of bound states n_{max} as calculated from Eq. (11) are given in Table (1). The calculations show that the estimation of the maximum number of bound states of the channeled positron for both armchair and zigzag are found to be n_{max} Ref.[14] > n_{max} (Moliere) > n_{max} (Universal), while for the case of chiral nanotube, n_{max} Ref. [14] = n_{max} (Moliere) and n_{max} (Ref. [14] and Moliere) > n_{max} (Universal).

Table (1): Values of the parameters a_1, b_1 and c_1 in Eq. (7) needed to fit the nanotube channeling potential calculated by using different potential models for the given (n,m) nanotubes, n_{max} is the maximum number of bound states for channeled positron with incident energy 100 MeV incident in a direction parallel to the nanotube axis.

(n,m)	Radius (nm)	Potential model	a_1 (eV)	b_1 (eV)	c_1 (nm^{-1})	n_{max}
(10,10)	0.673225	Ref..[14]	0.30951	0.0267	11.70454	20
		Moliere	1.08992	0.00149	16.85538	17
		Universal	1.00302	2.54126×10^{-5}	23.01093	12
(11,9)	0.674347	Ref. [14]	0.29904	0.0269	11.66859	20
		Moliere	0.29904	0.0269	11.66859	20
		Universal	0.52358	0.00227	15.08567	13
(18,0)	0.699636	Ref. [14]	0.29834	0.01793	11.84884	19
		Moliere	0.63897	0.00574	13.75914	18
		Universal	0.75919	1.54459×10^{-4}	18.8679	12

Table (2): The minimum potential, $U_{min}(\rho)$ (at the nanotube axis) and the maximum potential, $U_{\max}(\rho)$ (at the screening length from the nanotube wall) calculated by using different potential models and by Eq. (8) respectively for the given (*n*,*m*) nanotubes.

Potential model	(10,10)		(11,9)		(18,0)	
	$U_{min}(\rho)$ eV	$U_{\max}(\rho)$ eV	$U_{min}(\rho)$ eV	$U_{max}(\rho)$ eV	$U_{min}(\rho)$ eV	$U_{max}(\rho)$ eV
Ref. [14]	0.17266	55.5142	0.17057	55.5119	0.129503	55.4618
Eq. (8)	0.33621	52.5067	0.32594	52.3539	0.31627	52.9242
Moliere	0.17266	100.082	0.17057	55.5119	0.129503	70.4485
Eq. (8)	1.09141	82.8721	0.32594	52.3539	0.64471	61.6753
Universal	0.22807	88.5010	0.22621	43.8533	0.187988	58.9911
Eq. (8)	1.00305	76.0559	0.52585	40.8165	0.759344	52.1144

The minimum potential $U_{min}(\rho)$, (at the nanotube axis) and the maximum potential $U_{max}(\rho)$ (at the screening length from the nanotube wall) is shown in Table (2), for different nanotubes by using the channeling potential used in Ref. [14], and that by using both Moliere and Biersack's universal potentials. The values obtained by using the expression given by Eq. (8) which fit the above models are also given.

The obtained results of the energy eigenvalues of relativistic positron channeled through single-wall carbon nanotubes could be used in the calculations of the energy of the emitted channeling radiation. The emitted photon energy in the forward direction is given by $\hbar\omega = 2\gamma^2(\Delta E)$ where $\Delta E = E_{n+1} - E_n$ is the energy difference between the successive initial and final states of the channeled positron.

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