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Channeling of low energy atomic particles in carbon nanotubes with heterojunctions

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ABSTRACT

Low energy particle channeling through single-wall carbon nanotubes 245 nm long with (20,0)/(10,10) heterojunction has been studied. As demonstrated the ion beam cross-section becomes half the area after beam passage through the heterojunction.

1. Introduction

Previously the theoretical investigation of ion channeling in carbon nanotubes (CNT) [1] has been performed for three ion energy ranges [2]: high (E∼1 GeV) [3–11], medium (E∼1 MeV) [12–17] and low energies (E∼1 keV) [18–22]. Ion channeling in carbon nanotubes is a new and interesting research field due to three reasons: first, as there is an only one experimental work for CNT ion channeling [23], second, the ion beam manipulation by carbon nanotubes provides new opportunities for ion beam technologies; third, theoretical works for ion channeling in CNT, except [24] actually do not consider the impact of carbon nanotube defects. Channeling of low energy ions in carbon nanotubes was studied less than others. We consider investigation of low energy ion channeling in carbon nanotubes with defects to be of importance for further application in the ion beam technology. One of the unique defects peculiar only to CNTs is the heterojunction defect. The heterojunction (Fig. 1) has become one of the first defects studied after carbon nanotubes discovery [25]. Since, difference in diameters of carbon nanotube is determined by the temperature of synthesis process [26], the change of CNT diameter is achieved through the temperature variation at its synthesis. Indeed, as it is shown in the paper [27], the carbon nanotubes react to temperature alternation by including 5–7-defects in its structure. It gives cause to seamlessly connection of nanotubes with various chirality vectors. So, if CNT structure includes single 5–7-defect, the carbon nanotubes unite into heterojunction by the rule $(n,m)/(n\pm1, m\mp1)$, and if k 5–7 defects are integrated, the rule is as follows: $(n,m)/(n\pm k, m\mp k)$ [28]. Kink heterojunction can be formed by inclusion of separated 5–7 pairs (Fig. 1, C). The objective of this paper is to simulate ion beam passing through carbon nanotubes with a defect (20,0)/(10,10).

2. Methods

In the present paper we study channeling as a classic process based on the following arguments. We can consider an ingoing particle moving in the carbon nanotube of R radius as a wave packet with initial width δ_0. The wave packet width is increased during its motion in vacuum and therefore, at channeling within the void tube channel (see [29,30]):

$$\delta(t) = \sqrt{\delta_0^2 + \frac{t^2}{4\delta_0^2 m^2}},$$

where m is the mass of the particle, t is the time. Henceforward throughout the article Hartree atomic units $(e=1, m_e=1, \hbar=1)$ are applied in formulas.

However, in our case, an insignificant increase of the wave packet size is observed for the motion period of time from ∼10 to 100 ps. Furthermore, periodically localization of the wave packet occurs due to collisions with wall. In this way, the quantum

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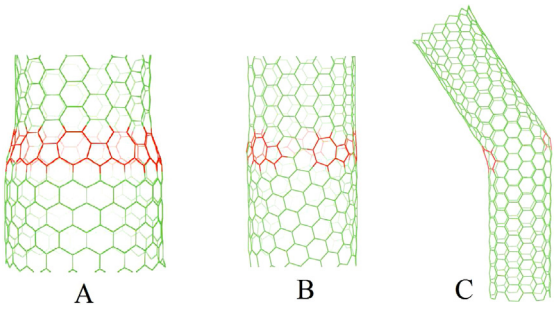

Fig. 1. Atomistic models of metal–semiconductor heterojunctions in single-wall CNT (A (20,0)/(10,10), B (15,5)/(10,10), C (7,7)/(12,0)).

mechanical spreading of the wave packet slightly affects the nature of the particle motion under considered conditions. Moreover, de Broglie wavelength of the channeling Ar^+ ion is approximately $10^{-4} - 10^{-3}$ nm, that is shorter than the interatomic distance in carbon nanotube, and the distance of closest approach at collision of Ar^+ ion–carbon atom is in $10^4 - 10^6$ times greater than de Broglie wavelength for the considered energies. Hence, it appears that quasi-classical method is applicable to our problem under consideration. We take into account that the quasi-classical quantum theory is also applicable here for describing purely quantum effects as diffraction or the self-capture in the own polarization well. If dealing with probability distribution of channeling particles, thus both theories, classic and quasi-classic, shall produce the similar results with minor deviations. In fact, when investigating phenomena in nano-structures (in so-called meso-structures), quantum and classic patterns are in the position of competitive ideas. As, rigorous quantum–mechanical phenomenon theory has not been formed heretofore the classic theory often has not alternative.

In our paper we had used LAMMPS program code [31], for the classical molecular dynamics (MD) simulation, and many-body potential AIREBO was used for description of interaction among carbons [32,33]. AIREBO is the semiempirical potential, taking into account atom hybridization, formation and destruction of interatomic bonds, and Van der Waals interaction among carbon atoms. For the interaction of the carbon nanotube atoms and Ar^+ ion Zieg ler–Biersack–Littmark-potential (ZBL) [34] has been applied. Besides ZBL-potential an electron stopping has been taken into account in the form of [18]:

$$F = -\frac{(Z_1^2\gamma\upsilon)}{(8\omega_s^2\rho^3)} - \frac{3(Z_1^2\upsilon)}{2\pi}\frac{\ln(0.692k_F\rho)}{(k_{TF}\rho)^4},$$

where Z_1 is the ion atomic number, υ is the longitudinal component of ion velocity, γ is the damping factor, ω_s is the surface plasmon frequency, ρ is the distance between ion and nearest carbon atom, k_F is the Fermi vector and $k_F = \upsilon_F = \pi k_{TF}{}^2/4$, where υ_F is the Fermi velocity.

The distance between Ar^+ ion and the nearest carbon atom to it located at the distance not exceeding the cutoff distance (r_s= 0.8 nm) which together with current value of the longitudinal component of ion velocity υ was used for calculation procedure of electron friction force. Provided that, the nuclear stopping has been considered within MD simulation procedure, the total stopping power has been taken into account.

The method of simulation cell periodic continuation has applied. The method lies in the fact of simulation cell periodic continuation with a new CNT fragment located along the nanotube common axis. Nanotube was divided into the fragments. Some of the fragments had defects, others – not. The fragments involved defects were closed by caps from both sides and the fragment being free of defects were placed into periodic boundary conditions for minimization of the edge effect perturbations [22]. Some of the fragments could be used repeatedly; in this case ion motion in the current fragment was accompanied by reset of carbon nanotube's atoms positions and velocities in the next fragment to the initial state, when the ion had passed the half of the current simulation cell along the nanotube axis. This method allowed to exclude non-physical interaction of the ion with CNT wall perturbation that could be contained in the fragment used before. Thereby, we take into account that ion velocity is 3–4 times higher than CNT wall perturbation propagation velocity [35]. During the transition from the tube defect-free fragment into a defective one, the ion is placed into the equivalent position with regard to the hexagonal CNT wall cell of nanotube. This procedure allowed to exclude additional non-physical perturbation of ion trajectory, which is conditioned by CNT fragmentariness. Method of simulation cell periodic continuation saves processor time and increases performance in several times as compared with the CNT simulation of full length.

Carbon nanotubes have been prepared for the calculations in few steps. Atom coordinates of each CNT fragment were generated at the first step [36], then, if nanotube fragment contained a defect, it was arranged into non-periodic boundary conditions. At the second step, geometric optimization of the nanotube potential energy was performed [37]. At the third step, random velocities of nanotube atoms were set in accordance with Gauss distribution at given CNT temperature. Thermostatic control was performed at the fourth step provided within 5 ps by Berendsen method [38], which allowed the system to reach required temperature with lowest fluctuations [39], then Nose–Hoover thermostat was applied during 5 ps [40,41], that made system's thermodynamic characteristics balanced with canonical ensemble at given temperature [39].

The initial positions of incoming ions in random manner had generated into the nanotube cross-section being perpendicular to its axis, cross-section diameter was chosen to be 10% less than CNT diameter. Ions possessed Gaussian initial energy distribution, random distribution through entrance angles α (Fig. 2) and azimuth entrance angle φ (Fig. 2)) distribution. Coordinate axes were directed in the way as shown in Fig. 2, CNT axis coincided with the z axis.

3. Calculation

The simulation was performed CNT 245 nm long at 300 K temperature.The first (input) nanotube 100 nm long consisted of fragment 1 is the CNT (20,0); the next 30 nm occupied defective fragment 2 is the CNT with heterojunction (20,0)/(10,10); the next 100 nm represented the fragment 3 is the CNT(10,10); the last

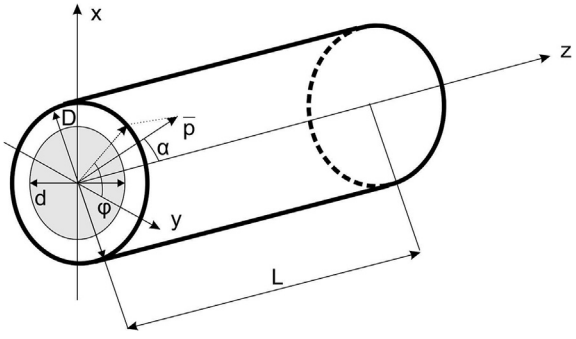

Fig. 2. Calculation pattern: D is the CNT diameter, d is the initial beam cross-section diameter, α is the initial angle between momentum $\vec{p}$ and nanotube axis (z axis), φ is the azimuth angle.

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