Channeling of heavy ions through multi-walled carbon nanotubes

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Abstract

Making use of molecular dynamics with analytical potentials we theoretically study channeling of heavy ions with keV energies through multi-walled carbon nanotubes. We show that under certain conditions on the tube alignment with respect to the ion beam and on ion energies, the ions can move through the empty cores of the MWNT with a very low probability of dechanneling. We further discuss how, by employing the experimental techniques routinely used nowadays for handling nanotubes on substrates, one can create a nanotube-based conduit for energetic ions, which should work as an aperture and allow one to manipulate the beam at the nanoscale.

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1. Introduction

Channeling of energetic ions through solids is a phenomenon which should be accounted for in the present-day semiconductor technology [1,2], as it gives rise to deeper implantation and less lattice disorder. The channeling effects are particularly important for materials with high crystallinity and anisotropic atomic structure. One can expect that the effective channeling of ions is possible in carbon nanotubes [3] (CNTs), as they have hollow cores, high aspect ratio and a low concentration of defects.

The motion of high-energy light ions (protons) through single-walled nanotubes (SWNTs) has received considerable attention [4,5]. The driving force for these studies was the possibility to use SWNT bundles for steering the beams of high-energy (GeV) protons, which would otherwise require cumbersome and expensive magnetic systems. However, despite an extensive theoretical analysis and first experimental results [6] it is not clear at all if CNTs can in practice be used for this
purpose, as the sample will quickly be destroyed by the beam as experiments on proton irradiation of SWNTs indicate [7].

Contrary to light ions, channeling of heavy ions through CNTs has not yet been studied. At the same time, this issue is of fundamental interest, as the well-controlled atomic structure of CNTs makes it possible to check (e.g. by the transmission electron microscope) the fundamentals of the channeling theory in general, and specifically in graphitic systems [8]. Besides this, as CNTs can easily be bent and manipulated at the nanoscale, developing a CNT-based conduit for energetic ions could facilitate the further progress in many applications, such as the solid-state quantum computing [9,10].

In this paper, we theoretically study channeling of heavy ions with keV energies through multi-walled nanotubes (MWNTs). We show that under certain conditions on the tube alignment with respect to the ion beam and on ion energies, the ions can channel through the empty cores of the MWNT with a very low probability of dechanneling.

2. Simulation method

To describe collisions of energetic ions with the nanotube, we employed molecular dynamics [11] (MD) with analytical potentials. To model carbon–carbon interactions, we used the Brenner II interatomic potential [12]. We chose Ar as the typical heavy ion. The interaction between Ar ions and C was modelled with the Ziegler–Biersack–Littmark universal repulsive potential [13]. A very large cutoff range of 4Å was used for the Ar–C interaction, as we found that shorter cut-off ranges effected the results. We did not account for the electronic stopping as the ion energies considered were low and the nuclear slowing down completely governed the collisional phase. Besides this, the electron density in the MWNT cores is very low. The simulations were carried out at zero temperature. Other details of the simulation methods can be found in our previous publications [14,15].

3. Results and discussions

Effects of ion irradiation on nanotubes have been studied both experimentally [7,16–18] and theoretically [19] (and references therein). When estimating the ion ranges, it has been assumed that the beam direction is perpendicular to the tube shells. Now, to address channeling through the tubes, we must consider the opposite case: the ion beam direction is nearly parallel to the tube axis, see Fig. 1.

To understand the nature of ion interactions with MWNTs, we considered first the collision of the ion with the inner shell of a MWNT, see Fig. 1. The neglect of all other MWNT shells is well motivated in this case as the shells are spatially separated by 3.2Å and they are only weakly bounded to each other via van der Waals-type forces [3].

We started with the following question: What happens during the collision of an Ar ion with a...
single-walled nanotube (SWNT) and how does the ion trajectory depend on the ion energy $E$ and the incidence angle $\Theta_1$ (the angle between the tube axis and the original ion velocity vector, see Fig. 1)? We considered ions with energies of 0.1–20 keV and $\Theta_1 = 8–20^\circ$. For each ion energy and angle we simulated 100 impacts and collected the statistics. The polar angle (the projection of the ion velocity vector onto the plane perpendicular to the tube axis) and the impact points were randomly chosen. In this work we considered (17,0) zigzag SWNTs with a diameter of about 1.3 nm.

We found that at low energies the ion is always bounced back by the wall and it remains inside the core region without creating any damage to the tube, but giving rise to pressure waves and local heating. At higher energies the ion can sputter 1–4 carbon atoms from the tube, but it still remains inside the tube. At a certain energy $E_{dc}$ (the dechanneling energy – the maximum energy for channeling) which depends on $\Theta_1$, the ion goes through the wall, as one can expect from the momentum and energy conservation laws. The probability of dechanneling (the number of dechanneled ions per incident ion) as a function of ion energy is shown in Fig. 2 for the zigzag SWNT. It is seen that $E_{dc}$ is critically dependent on the angle, but even when the ion energy is higher than $E_{dc}$, the ion has a finite probability to stay inside the tube after the collision. This is related to different local geometries at the impact points and thus different ways of momentum transfer to the tube atoms.

Using the data given in Fig. 2, one can plot $E_{dc}$ versus the angle, or the other way around, one can present the maximum, or critical, angle $\psi_c$ as a function of ion energy, see Fig. 3. The simulations results shown in Fig. 3 can be described by a universal curve fit to the data. We found that the results can well be reproduced by an equation

$$\psi_c = \text{const}/\sqrt{E},$$

see also Fig. 3. This is in line with a general equation [1]

$$\psi_c = \sqrt{U(r_c)/E},$$

where $U(r_c)$ is the ion potential energy at the critical approach distance $r_c$. This equation has been derived within the framework of the continuum theory of channeling. Note that Eq. (2) is of limited validity (see e.g. [1] and references therein), as only one row or plane of atoms is taken into account to calculate $\psi_c(E)$. However, the open
structure of SWNTs motivates well this approximation, as our simulation data obtained with account for the interaction of the ion with all C atoms within the cutoff range indicate.

The next highly important issue to be addressed is the average scattering angle $\Theta_2$ of the ion, see Fig. 1. One can expect that an ion propagating through the MWNT core will collide many times with the inner wall of the MWNT. Thus, if $\Theta_2$ grows after each impact, this should inevitably result in ion dechanneling. On the contrary, if $\Theta_2$ decreases, after several collisions the ion trajectory will be nearly parallel to the tube axis thus decreasing the probability of dechanneling.

We found that for slow ions the ratio $\Theta_2/\Theta_1$ is higher than unity, which corresponds to ion defocusing. However, at a certain crossover energy $E_{foc}$ the ratio $\Theta_2/\Theta_1 < 1$, which means that, the other way around, every collision should decrease the angle. Energy-related changes in the ratio $\Theta_2/\Theta_1$ can be understood within the binary collision approximation: the impinging particle scattering can be understood within the binary collision approximation: the impinging particle scattering angle can be arbitrary small. In reality, this means that the averaged angle will fluctuate around the value corresponding to $E_{foc}$ in the diagram.

Having analyzed propagation of energetic ions through SWNTs, we moved on considering effects of the high-dose irradiation on the atomic structure of a MWNT composed of (10,10), (15,15) and (20,20) SWNTs. Details of these simulations will be published elsewhere [20]. We found that although the open end of the tube quickly becomes completely amorphous, the inner core remained open up to a dose of $\Phi = 4 \times 10^{15}$ cm$^{-2}$. This means that MWNTs, especially the MWNTs with larger inner cores can survive “shooting” about hundred ions before the end of the tube is com-
pletely destroyed and closed. Note that a substantial part of defects in the MWNT should anneal due to the migration of carbon interstitials [21] and by saturating vacancy dangling bonds [15].

The efficient channeling of ions through MWNTs can be employed to make a MWNT-based apertures to steer the ion beam. Such an aperture can be produced by using a combination of techniques routinely used nowadays for handling supported CNTs. A MWNT deposited on a substrate can be straightened [22] and cut [23] to open its ends by the tip of the atomic force microscope, then by applying a combination of etching and electron-beam lithography techniques [24] the metal shield can be produced. The beam can be steered by moving the whole unit or, ideally by bending the MWNT. Thus, the target can be irradiated in predetermined positions by a beam just several nm across. Such a device can be used for implanting ions or even single ions, which is highly important for the further progress in the solid-state quantum computing [9,10].

4. Conclusions

To conclude, we theoretically studied channeling of Ar ions through MWNTs. We found that the ions can channel through the empty cores of the MWNT with a very low probability of dechanneling. We showed that the dependence of the critical angle on ion energy obeys a simple universal equation and the continuum theory of channeling should work well in nanotubes due to their open structure. As interactions of energetic ions with the target can well be described by the universal repulsive potential [13] such a behavior should be general not only for Ar but also for other heavy ions. We finally suggested a nanotube-based conduit for energetic ions, which should work as an aperture and allow one to manipulate the beam at the nanoscale.

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