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Energy distribution of the particles obtained after irradiation of carbon nanotubes with carbon projectiles

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ABSTRACT

The idea of using carbon nanotubes (CNTs) as masks against irradiation has recently emerged, because of the region of a given material covered by a CNT can be protected from the effects of irradiation, creating nanowires. In this case, it is interesting to know in detail the number of generated recoils and their energy. In order to obtain these data, we simulate the irradiation of CNTs with carbon ions using a molecular dynamics code. To describe the interaction between carbon ions we use the Brenner potential joined smoothly to the Universal ZBL potential at short distances.

We have analyzed the energy distributions of the carbon atoms emerging from the CNT for single projectile irradiation with incident energies from 30 eV to 5 keV. Our results show that the number and the energy of the recoil carbon atoms emerging from the CNT increases with the projectile incident energy. In average, each projectile with incident energy of 1 keV produces ~3.6 recoils, which have a mean energy of 150 eV, while projectiles with 5 keV produce ~7 recoils with a mean energy of 400 eV.

1. Introduction

The interest in the study of carbon nanotubes (CNTs) has been increasing since their discovery in 1991 [1]. This is due to the outstanding electronic [1], mechanical [2] and even magnetic properties [3,4] discovered in the CNTs. For instance, it is known that the CNTs may be conductors or semiconductors depending on their chirality [1]. Some recent advances in the manufacturing of CNTs with a given chirality [5], suggest that in the near future CNTs may be ideal candidates for use in nanoelectronics. There are other exciting potential applications of CNTs as well [1,2]. The ion irradiation of CNTs by light ions has also been thoroughly studied in the last years because the defects generated by the irradiation and the subsequent reconstruction are able to change the CNT's properties in a controlled way [6,7]. Moreover the irradiation can modify the structure of the CNTs, create junctions between them, or weld them [6].

Lately, the idea of using CNTs as masks against irradiation has emerged. In this way the region of the substrate covered by the CNT can be protected from the effects of irradiation [8,9], creating nanowires of a given material. For this kind of applications, and others where the projectiles interact with another material after the interaction with the CNT, it is interesting to know in detail the number of generated recoils and their energy distribution as well.

In this paper, we study the energy distributions of the particles obtained after irradiation of a single-walled CNT with carbon projectiles, distinguishing the contribution of both projectiles and recoils. We will analyze a range of projectile energies going from 30 eV up to 5 keV using simulations based on a molecular dynamics code in order to study the effect of the CNT bombardment.

2. Simulation method

We have developed a numerical code based on classical molecular dynamics (MD) [10] in order to simulate the irradiation of CNTs by carbon projectiles with incident energies ranging from 30 eV to 5 keV. It is worth to mention that we have neglected the electronic energy-loss in our simulations because of the low projectile energies involved in this work.

The forces acting on each particle were modeled by means of empirical interatomic potentials. We describe the C—C interactions using the Brenner potential [11], but without considering the time-consuming bond conjugation terms. It is worth to mention that we are interested in the energy of the particles emerging from the CNT, which means that the projectile must transfer more than ~25 eV to an atom of the CNT. In these relatively hard collisions the bond-conjugation terms of the Brenner potential are not

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relevant. In order to describe realistically close collisions the Brenner potential was smoothly linked [12] to the Ziegler–Biersack–Littmark (ZBL) universal potential at short interatomic distances [13].

We have used the velocity Verlet algorithm [14] to numerically solve the equations of motion of all interacting atoms. To improve the computing time, our code uses a variable time step Δt which depends on the maximum velocity and force.

In order to avoid the displacement of the CNT during the irradiation with carbon projectiles, we have kept fixed the atoms at both ends of the CNT during the simulation. The CNT temperature is controlled using the Berendsen thermostat [15].

We have studied in our simulations a single-walled CNT, armchair (10, 10), with length ∼100 Å, radius $r_{\mathrm{CNT}} \sim 7$ Å, and with its axis parallel to the z-axis. We show in Fig. 1 the CNT, which is attached by its ends, so both ends have fixed positions. The velocity of the carbon atoms located in a region of 5% of the total length of the CNT, next to its fixed ends, are scaled according to the Berendsen thermostat, as previously mentioned. The carbon projectile bombards the CNT in the direction perpendicular to the nanotube axis, although the exact impact coordinates are randomly distributed on a central region of 10% of the total length of the CNT.

We simulate the bombardment of the CNT with one carbon projectile with incident energies from 30 eV to 5 keV and evaluate the dynamics of the system during 2 ps, with a thermostat temperature of 300 K.

The main damage mechanism during bombardment is the transfer of energy from the projectile to the CNT, which results in the displacement of the atoms of the CNT structure, resulting on vacancies generation. Depending on the transferred energy, the primary atoms can be backscattered, replace or extract atoms of the CNT, or even they can be added to the structure (adatoms). Using our simulation code, we have obtained the energy distributions of the carbon atoms emerging from the CNT, both primary atoms and recoils. Such information could provide information about the damage produced on the substrate behind the CNT, when using these as mask against irradiation.

3. Results and discussion

We show in Fig. 2 the number of carbon atoms per incident projectile emitted from the CNT as a function of the projectile incident energy E_0. The blue circles correspond to particles originally belonging to the CNT, i.e. recoils, while the red squares indicate the number of projectiles which emerge from the CNT after the interaction. The number of nanotube recoils generated per projectile increases with the incident energy, being ∼7 for 5 keV. Analogously, the number of projectiles that traverse the CNT also increases with the incident energy, being most of them projectiles for 5 keV incident energy. It is worth to mention that, although a saturation effect is observed in both situations, the limit values are not reached with 5 keV incident energy.

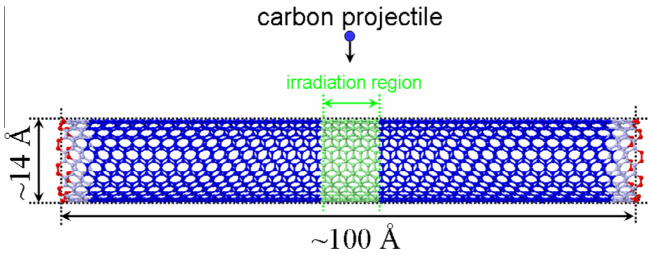

Fig. 1. Armchair (10, 10) single-walled CNT irradiated by carbon projectiles. Red atoms at both ends are fixed, grey atoms close to both ends act as a Berendsen thermostat. Carbon projectiles bombard the central region of the thermostat represented by green atoms. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

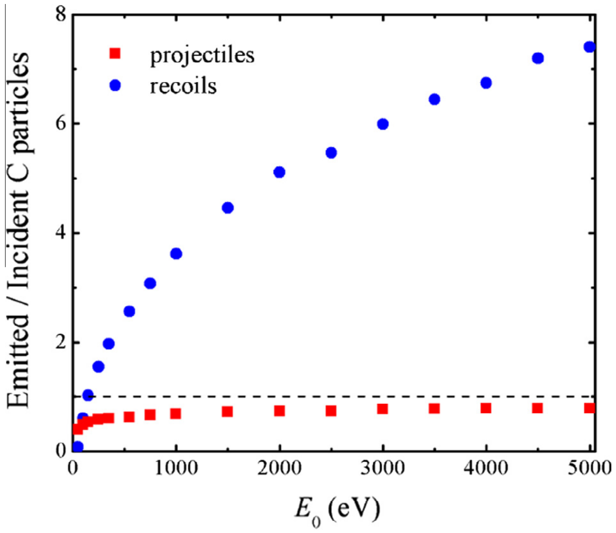

Fig. 2. Number of particles which are emitted from the CNT after bombardment as a function of the incident energy of the carbon projectile. The blue circles correspond to particles originally belonging to the CNT, while the red squares indicate the number of projectiles which emerge from the CNT after the interaction. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

When using CNTs as protection mask against irradiation, the energy distribution of the carbon atoms traversing the CNT can provide useful information to determine the damage produced on the substrate. In Fig. 3 we have depicted the energy distribution of the carbon atoms traversing the CNT after irradiation with projectiles with different incident energies. Thin red curves represent the energy distribution of the carbon recoils, thin black curves are the energy distribution of the incident projectiles, and thick black curves represent the corresponding sum, i.e. the energy distribution of all particles traversing the CNT. It is important to highlight that particles with energies lower than 50 eV do not produce significant damage in the substrate below the CNT; even if those low energy particles give rise to a displacement of surface substrate atoms, this damage should anneal easily [9].

It is interesting to note that for all the projectile incident energies analyzed in this work, the energy distributions of the emitted particles show relative maxima around ∼15 eV, as can be observed in Fig. 3. Considering that only particles with energies higher than 50 eV can produce damage on the surface of the substrate [9], this suggest that using CNT can be effective as protection masks. The relative maxima around ∼15 eV is mainly due to carbon recoils, whereas the relative maxima observed around E_0 is due to the incident projectiles. Specifically, the latter can be associated with the projectiles that hit the CNT near its border. In order to clarify this, we have depicted in Fig. 4 the energy distribution of the particles emitted after irradiation with 50 eV projectiles that hit the CNT with different impact parameters b. For projectiles hitting the CNT with impact parameters $b > 1.1r_{\mathrm{CNT}}$, most of the particles emitted are projectiles, as observed in Fig. 3, which lose a small amount of their energy, because of the weakness of the interaction with the CNT wall. On the other hand, the particles emitted when the projectiles hit the CNT with impact parameters $0.9r_{\mathrm{CNT}} < b < 1.1r_{\mathrm{CNT}}$ are both projectiles and carbon recoils. In this case, the projectiles lose more energy during interaction with the CNT wall, which gives a maximum around ∼35 eV in the corresponding energy distribution. Finally, almost all particles emitted after irradiation with projectiles with impact parameters $0 < b < 0.9r_{\mathrm{CNT}}$ are carbon recoils, which have a maximum around ∼15 eV.