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# Stopping of energetic ions in carbon nanotubes

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## Abstract

Making use of empirical potential molecular dynamics, we simulated the bombardment of single-walled carbon nanotubes with various ions. We calculated the irradiation-induced damage which proved to be higher for heavy ions than for light ones due to higher values of the cross-section for the defect production in a nanotube. We demonstrated that chemical aspects of ion–nanotube interactions and finite temperatures are of minor importance when energetic ions penetrate through nanotubes. We finally estimated the ability of nanotubes to stop energetic ions.

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## 1. Introduction

Experiments on the irradiation of carbon nanotubes with energetic particles have revealed many interesting phenomena. The examples are irradiation-induced carbon nanotube coalescence [1], welding [2] and cross-linking [3], just to mention a few. These effects may potentially be used in various practical applications, such as nanotube-based reinforcement materials or nanoelectronics. Besides this, ion bombardment and carbon nanotubes as masks can be employed for fabricating ultra-narrow metal nanowires of about 10 nm in width [4].

Because it is conceptually possible to position carbon nanotubes quite accurately on a substrate using an atomic force microscope by pushing them mechanically [5], they may also be used for spatially selective ion implantation, especially for low-energy (a couple of keV) applications [6]. After irradiating a sample having a nanotube network on the surface, ions will be implanted everywhere except for the regions below the nanotubes provided that the nanotubes are thick enough to stop the ions.

Reasoning from the data on Ar ion irradiation [7–9] of single-walled (SWNTs) and multi-walled (MWNTs) nanotubes, it is clear that only the latter could be used to effectively stop keV-ions. However, to understand the basic physics of damage creation and stopping ions of different types, it is instructive to dwell first upon the irradiation of SWNTs due to their simple and well-defined structure. The main goal of this work is to find out

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how the damage production in SWNTs depends on the mass of incident ions.

## 2. The simulation method

In order to simulate impacts of energetic ions onto SWNTs, we made use of molecular dynamics [10] with empirical potentials. To model the carbon–carbon interaction (for carbon atoms in the SWNT and when the incident ion was also carbon), we used the Brenner II interatomic potential [11] smoothly joined at short interatomic separations with a repulsive potential calculated by a density-functional theory method [12]. The joining to the equilibrium potential was done using a Fermi function, with the parameters given in [13]. The interaction between noble-gas ions and C was modelled with the Ziegler–Biersack–Littmark universal repulsive potential [14]. The Si–C interaction was described by the ZBL potential as well. This potential does not take into account the chemistry of Si–C interaction, but the chemical aspects are not important for the range of energies considered (50–500 eV), which are much higher than the Si–C bond energy. Notice also that, in this work, we are primarily interested in stopping power of the SWNT, but not in defects which appear under ion impacts.

Berendsen temperature control [15] was used at the borders of the SWNT. 10-nm-long SWNTs were considered. The impact points were randomly chosen over the central part of the nanotube with a width corresponding to the nanotube diameter. The energy range of incident ions was between 50 and 500 eV. For every ion energy considered, we carried out 400 independent runs and averaged the results. Visual analysis was employed to understand whether the ion penetrated the SWNT or not. We estimated the ion energy lost in an impact as the difference between the initial and final ion energies.

## 3. Results and discussion

Our simulations showed that, for all the ions considered, the irradiation resulted in the sputter-

ing of carbon atoms from the SWNT and formation of vacancies on the SWNT walls. Single- and multi-atom vacancies were the most common defects. Since the knowledge of the number  $N_r$  of recoils below a nanotube is important for preventing ion implantation in the substrate below the nanotube, in Fig. 1 we show  $N_r$  (both ions and C atoms) as a function of incident ion energy  $E_i$  for different types of the ions. We defined  $N_r$  as the number of particles which crossed an area below the SWNT with the same width and length as the nanotube dimensions.

It is seen from Fig. 1 that recoils appear at a certain energy (about 50 eV). Then  $N_r$  grows up with energy up to  $E_i \sim 0.3$  keV, after which  $N_r$  approaches a value which depends on the ion mass. These results were calculated for a (10,10) armchair SWNT. Simulations on SWNTs with different chiralities gave the same results within the statistical uncertainties. The analysis of the recoil energies showed that ions (except He) lose on the average 0.3 keV of their kinetic energy when penetrating a SWNT.

Except for noble-gas ions, we considered also C ions to see if chemical aspects of ion–nanotube

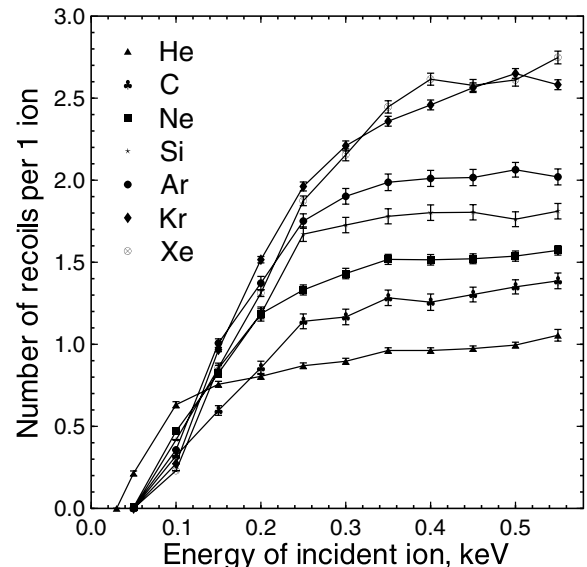


Fig. 1. Number of energetic recoils (both incident ions and C atoms) below single-walled nanotubes as a function of incident ion energy for various ions.

interactions are important in ion stopping. It is evident that the C simulations are consistent with the general tendency: the number of recoils grows up with the ion mass.

The behavior of ion-induced damage in SWNTs is in line with the number of recoils. In order to quantitatively characterize the damage, we plot in Fig. 2 the number of C atoms in the SWNT with a coordination other than three as a function of ion energy (in a perfect nanotube all carbon atoms have three neighbors). The amount of damage increases quickly with  $E_i$  for low ion energies, then it grows more slowly or even drops for light ions.

This behavior can be understood in terms of the cross-section for the defect production in a SWNT. We estimated the cross-sections for different ions by calculating the maximum impact parameter for which an ion transfers at least 25 eV (the threshold energy for displacing an atom in the nanotube) to a C atom in a binary collision (see Eqs. 2-62, 2-64 in [14]). The cross-sections  $\sigma$  ( $\sigma = \pi p^2$  where  $p$  is the impact parameter) for various ions are presented in Fig. 3. It is evident that the cross-section for He is very low, which explains the low number of defects created by He

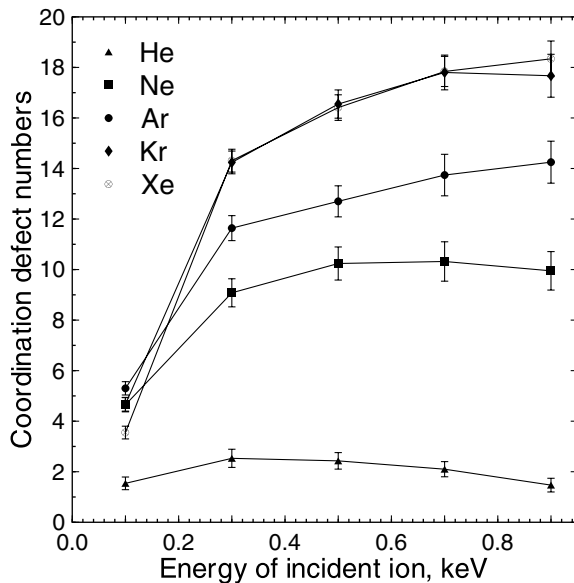


Fig. 2. Average coordination defect numbers in single-walled nanotubes (the total damage) as a function of incident ion energy.

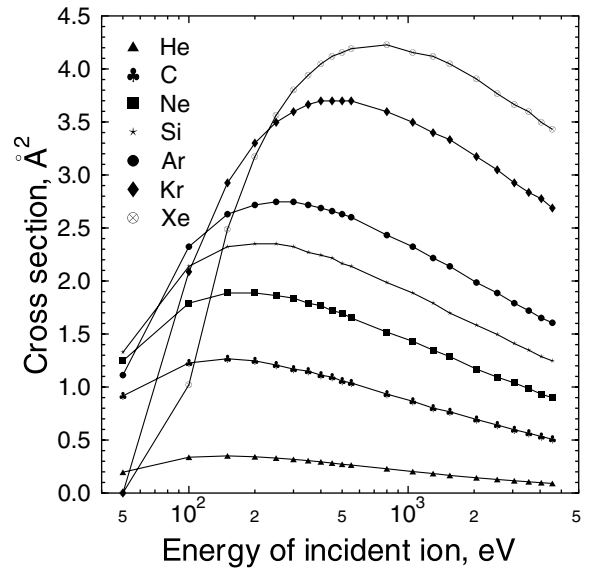


Fig. 3. Cross-section for the defect production in nanotubes as a function of incident ion energy for various ions.

ions. The maximum in the cross-sections moves to higher energies with increasing ion mass. Thus, in the energy range from 0.2 to 0.7 keV, the averaged cross-section for Kr and Xe ions is roughly the same, which is why the damage created by these

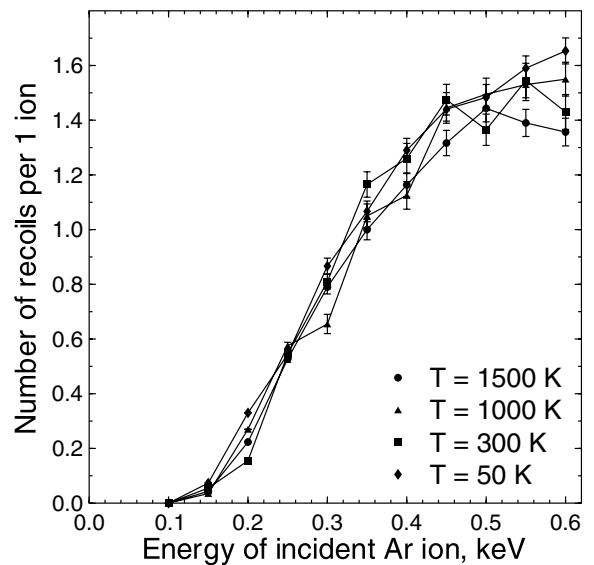


Fig. 4. Number of energetic recoils as a function of incident Ar ion energy at different temperatures.

ions is approximately equal in the energy range considered.

All the impact simulations were carried out at 0 K. In order to see how the temperature affects the number of recoils, we simulated argon irradiation at temperatures of  $T = 50, 300, 1000, 1500$  K.  $N_r$  as a function of  $E_i$  is shown in Fig. 4 at these temperatures. It can be seen that the behavior at different temperatures is quantitatively the same. Hence, we can conclude that temperature effects are not significant for the primary damage production in carbon nanotubes.

#### 4. Conclusions

In this paper, making use of molecular dynamics, we simulated low-energy irradiation of SWNTs with various ions. We found that, for all the ion types considered, the most prolific defects are vacancies on the nanotube walls. For one and the same ion energy (larger than 0.3 keV), the total amount of the irradiation-induced damage is higher for heavy ions due to higher values of the cross-section for the defect production in a SWNT.

We also estimated the ability of SWNTs to stop energetic ions. Chemical interactions between nanotubes and ions and finite temperatures were demonstrated to be of minor importance when energetic ions penetrate through nanotubes. We found that at energies less than 1 keV, ions lose about 0.3 keV of their kinetic energy in a collision with one shell. Thus, given that MWNTs usually have tens of the graphitic shells, they can easily stop energetic ions with energies up to 10 keV and thus can be used for spatially selective ion implantation. Future studies will quantify these qualitative conclusions.

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