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Bonding effect on channeling of C ions in a carbon nanotube

LI Yong ZHANG Wei XU Zijian* ZHENG Liping ZHU Zhiyuan HUAI Ping

Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China

Abstract The channeling phenomenon of carbon ions in single-wall carbon nanotubes (SWCNTs) is investigated by using the molecular dynamics simulation with analytical potentials. The relationship between the channeling critical angles in the SWCNT and the bonding interaction is analyzed. It was found that, at 200–5000 eV and 10°–20° of incident angle, the ions with the bonding interaction or chemical effect, have decreased dechanneling probabilities and increased critical angles, compared to that of non-bonding ions. So the bonding effect cannot be ignored in the channeling mechanism of carbon ions through a SWCNT.

Key words Channeling, Bonding effect, Carbon Nanotube, Molecular dynamics

1 Introduction

With unique electronic, mechanical and thermal properties, carbon nanotubes (CNTs) are among the most prospective candidates for building nanometer-scale electronic and mechanical devices, and a variety of CNT-based functional materials. The hollow cylindrical structures of CNTs, combined with their superior mechanical strength, high chemical stability, high aspect ratio and a low concentration of defects, suggest a potential application of nanotubes: steering energetic charged particles that are passing through the cylindrical channel of CNTs.

There have been a number of molecular dynamics (MD) simulation investigations on channeling of particles through CNTs. Krasheninnikov A V and Nordlund K[1,2] used MD simulation first to study the channeling motion of heavy ions through multi-walled CNTs(MWCNT), and demonstrated that the dependence of critical angle on ion energy could be described by a simple equation Moura C S and Amaral L[3,4] investigated the dependence of maximum projected range on energy at the critical incident angle, and the transport characteristics of ions in CNT ropes. Previous Monte Carlo and MD simulations[5-8] showed that the ion mass effect is important to the critical channeling behaviors and gave a theoretical expression for the critical angle including mass and charge of incident particles channeling in a single-walled CNT (SWCNT) or its rope at low energies.

In our latest MD simulation research[8], we confirmed that mass of the incident ion is an important factor for ion channeling through SWCNTs by using the universal Ziegler-Biersack-Littmark (ZBL) repulsive potential[9]. However, when the incident ion is chemically active, the bonding interaction should be taken into account in the simulation of channeling, and it is not enough to use just the repulsive screened Coulomb potential. In this paper, we report our MD investigation on the C ions propagating through (10, 10) SWCNTs, considering the bonding interaction of incident C ions with CNT atoms. The simulation results were compared with hypothetical C ions without bonding action, which are referred as "Cn" ions (n stands for no bonding effect). It was found that, for 200–5000 eV C ions at incident angles of 10°–20°, the bonding interaction plays an important role in the channeling process.

2 Computational details

Classical molecular dynamics (MD) with analytical potentials is used to simulate C and "Cn" ions channeling through a (10, 10) armchair SWCNT, using a MD code developed by our group and having been

* Corresponding author. *E-mail address:* xuzijian@sinap.ac.cn

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applied successfully to mechanisms of the ion-induced damage to CNTs[10,11]. The SWCNT is 120 Å in length. The second generation of the reactive empirical bond-order potential[12] (REBOII) was used to model the covalent interatomic interaction of the SWCNT. To model the close-range collision realistically between the incident C ion and the SWCNT atoms, the bonding potential of REBOII is smoothly splined to the ZBL universal repulsive potential at short interatomic distances using a Fermi function. The "Cn"-C interaction is only described by the ZBL potential and a cutoff range of 4 Å is used. The electronic stopping is not taken into account because the C ions are just of 200–5000 eV, where nuclear stopping governs the collision.

The equations of motions are solved by using the velocity-Verlet algorithm. In the simulation, the time step is allowed to vary depending upon the maximal velocity and potential energy of the atoms [13]. The time step is determined as

$\Delta t_n=0.05\text{Å}/\{\max_{1\le i\le N}[2E_{ki}/M_i+2\max(0, E_{Pi})/M_i]\}^{1/2}$,

where E_{ki}, E_{Pi} and M_i are the kinetic energy, potential energy and mass of the i^{th} atom, respectively; and N is the total numbers of atoms of the armchair SWCNT. This method of variable time steps has been used in the investigation of irradiation-induced damage production in CNTs with different diameters and chiralities[10] and by several types of ions[11]. As in our previous work[8], we set the incident directions nearly parallel to the tube axis. The chosen number of time steps is large enough to simulate the whole process of ions propagating through the SWCNT. In each channeling event, the propagating process is deemed as finished when the incident ion penetrates the tube wall or gets out from the other end of the SWCNT.

3 Results and discussion

In this study, the C and "Cn" ions transporting through the (10, 10) SWCNT are of 200–5000 eV in initial energy and 10°–20° in incident angle The dechanneling probabilities as a function of ion energies and incident angles are shown in Fig.1.

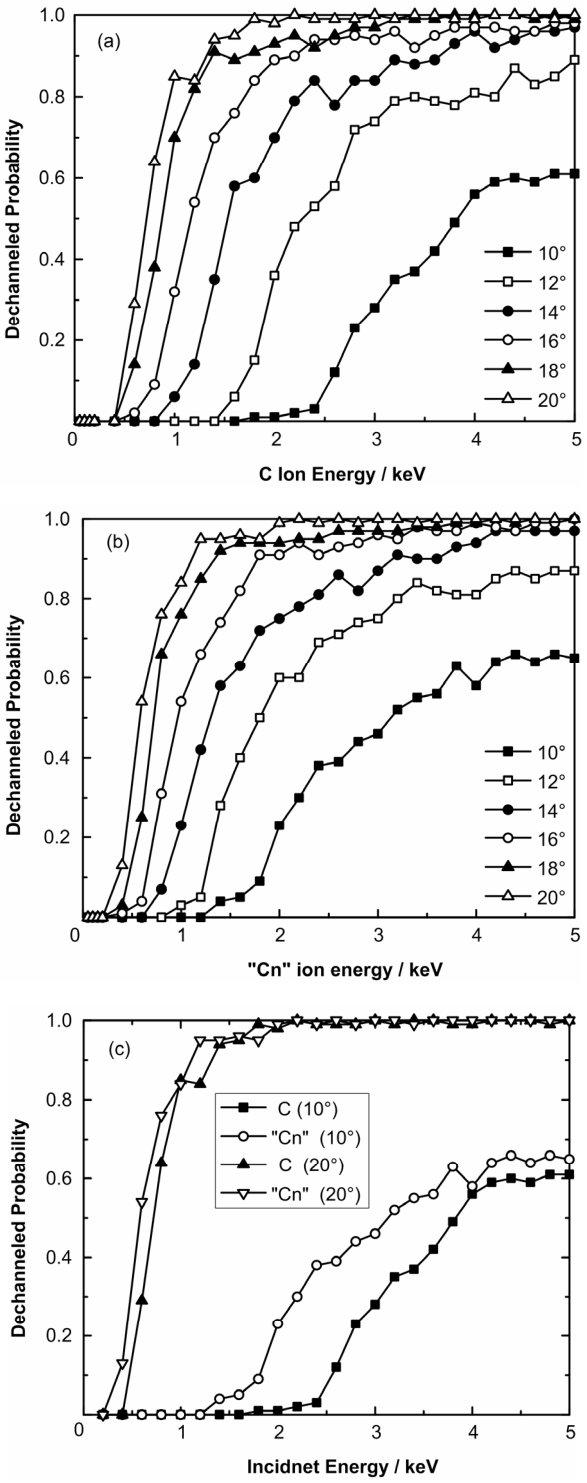

Fig.1 Dechanneling probability of ions in different incident angles, as a function of incident energy, for C (a) and "Cn" (b) in an armchair (10, 10) SWCNT, and dechanneling probabilities for C and "Cn" at incident angles of 10° and 20°(c).

The dechanneling probability is very low at low energies, and rises abruptly at certain incident energy, e.g. 600-eV "Cn" ion at incident angle of 16°. And it increases with incident angle. Although the dechanneling probabilities of C and "Cn" ions vary

similarly with the energy and incident angle, it can be seen evidently that the dechanneling probability of "Cn" ions is significantly higher than that with the bonding effects, especially at smaller incident angles (Fig.1c). In other words, the bonding interaction reduces the dechanneling probability of the incident ions, which results in larger channeling critical angles for ions with chemical effects, as shown in Fig.2. The critical channeling behavior of "Cn" ions is homologous to that of inert ions such as He, Ne, Ar and Kr[8]. In this context, one sees that, besides the ion mass effect, the chemical interactions of B, C, N, Si, etc with CNT atoms play an important role in channeling mechanism of CNTs.

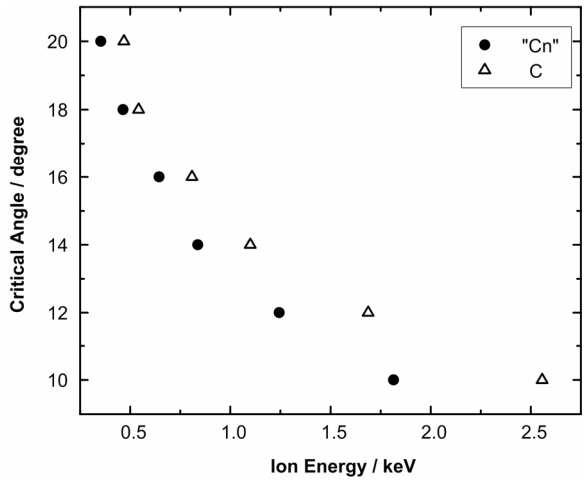

Fig.2 Channeling critical angles of C and "Cn" ions as a function of incident energy. The critical angle is determined at the dechanneling probability of 0.1.

In research for mechanisms of the bonding-effect-induced differences between the C and "Cn" channeling behaviors in SWCNT, we analyzed the dynamical processes and potential function curves in the two cases. The channeling trajectories and kinetic energy of C and "Cn" ions are shown in Fig.3.

As shown in the insert in Fig.3, a carbon ion without the bonding interaction penetrates out of the tube, while the ion with the bonding interaction channels well, though the two ions are of the same initial position and velocity. From the kinetic energy in Fig. 3, one sees that in the first knock on the tube wall, a "Cn" ion loses or transfers more energy to the atoms nearby CNT wall than a C ion. This is due to the more violent knock and longer knock-on time in the ZBL potential case than in the Brenner-ZBL combination potential case.

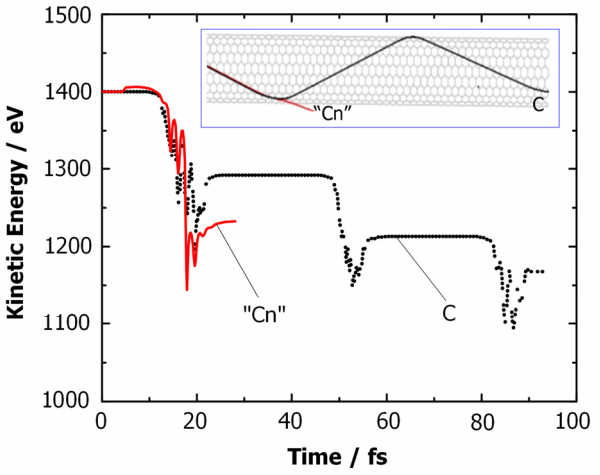

Fig.3 Kinetic energy of the incident ion as a function of simulation step number in one channeling event at 1400 eV and incident angle of 16º. The insert shows the trajectories for C and "Cn" in the SWCNT.

We compare the two kinds of incident ion interactions with CNT wall in Fig.4. When the ZBL potential is combined with the Brenner potential using a Fermi function, the resultant repulsive part around 1 Å interatomic distance is steeper than the pure ZBL repulsive potential (Fig.4a). This steeper potential makes the repulsive force wall of bonding potential shifted far away from the target atom center relative to that of ZBL potential (Fig.4b), and this outward shift of repulsive wall also makes the incident ion collide or knock with more target atoms simultaneously. As the attractive part of bonding potential does not transfer energy from the ion to the targets in a collision, the energy loss from an incident C ion is dispersed into relatively more C atoms of the SWCNT, while the energy loss from an incident Cn ion is focused into relatively less CNT atoms, hence the occurrence of a violent knock being well capable of cracking the wall in a non-bonding ion incidence.

Also, as the attractive interaction does not induce energy transfer from the ion to the targets, and the repulsive force wall is shifted outward in the bonding potential for an incident "Cn" ion, the interatomic distance range for energy transfer from an C ion to the target is much shorter than that of a "Cn" ion. Considering the incidence condition of near parallel to the CNT axis for channeling motion, the effective knock-on time for an incident "Cn" ion is longer than that for an incident C ion in a collision event.

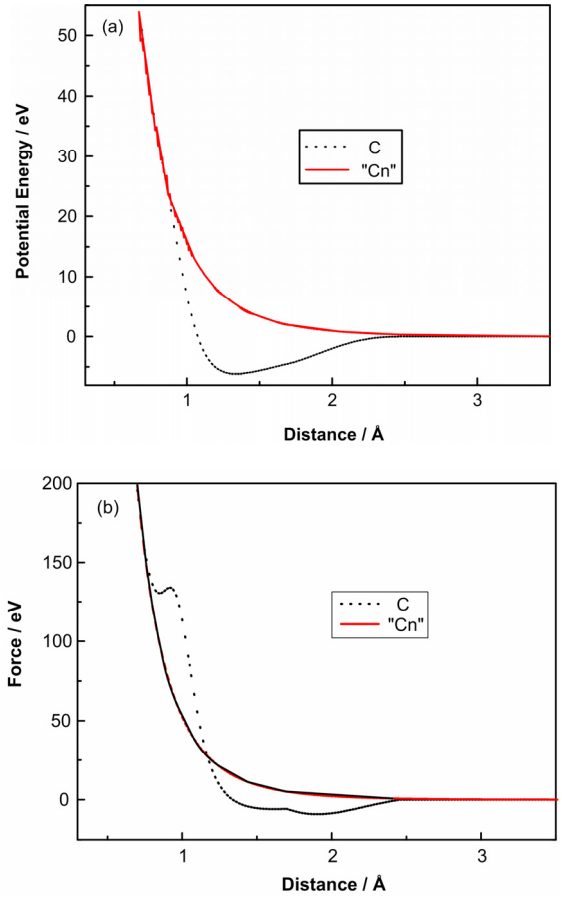

Fig.4 The potential energy (a) and force (b) curves as functions of interatomic distance, for both C and Cn interactions with a CNT atom.

Due to the two reasons above, the dechanneling probability of a C ion with bonding effect is lower than that of an ion without bonding effect, and accordingly, the channeling critical angles of bonding ions are larger than that of non-bonding ions in the SWCNT. In fact, the difference between the two kinds of ion interactions with the targets is due to different distributions of electron clouds around the atom cores. When the ion is close to a target atom, for a bonding ion, its electron clouds are anisotropically distributed with one or several cloud branches towards the nearest target atoms, while for a non-bonding ion such as Ne and Ar, its electron clouds are still isotropically or spherically distributed, without significant changes.

4 Conclusion

Using the MD method with analytical potentials, we study the channeling mechanism in SWCNTs with the incident ions that are different in the bonding property of interaction with CNT atoms. Our simulation results show that, in the energy range 200–5000 eV, the bonding interaction between the incident ion and carbon atoms of the CNTs can significantly reduce the dechanneling probability, and accordingly, increase the channeling critical angle of this ion with bonding effect. We believe that the bonding interaction or the chemical effect of incident ions cannot be ignored in the channeling process of C-like ions (B, N, Si, etc) through CNTs. These results will be helpful for better understanding the channeling mechanism with different kinds of ions passing through the SWCNTs.

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