ON PARTICLE IMPACT INDUCED BOND BREAKING OF SINGLE-WALLED CARBON NANOTUBES

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Introduction

Injection of particles to the side wall of single-walled carbon nanotubes (SWCNT) has been employed for doping and storage of particles on SWCNTs [1]. In addition, particle bombardment can be used to cut and modify graphene structures [2]. While the collision of hydrogen atoms with SWCNTs has been extensively studied [3], collision dynamic behavior of heavy particles with SWCNTs has not been well understood. To facilitate a better understanding of the particle-SWCNT collision process, in this work, we study the impact of five noble gas atoms (He, Ne, Ar, Kr, Xe) with SWCNTs and investigate particle impact induced CNT bond breaking phenomena. Simulation results include the bond-breaking kinetic energy ranges of the incident atoms with reflection and penetration after the collision. Effect of chirality of the SWCNTs and energy exchange between the incident atoms and carbon atoms of SWCNT are investigated.

Simulation Method

Collision of noble gas atoms (He, Ne, Ar, Kr, Xe) with single-walled carbon nanotubes of zig-zag type is studied using classical molecular dynamics simulation method. Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [4] is used for the interactions between the carbon atoms of the nanotube. The interaction between CNT and noble gases is described by Lennard-Jones (LJ) potential. The parameters for gas-carbon interaction are obtained from the Lorentz-Berthelot rule:

$$\sigma_{GC} = \frac{\sigma_{GG} + \sigma_{CC}}{2} \qquad \epsilon_{GC} = \sqrt{\epsilon_{GG} + \epsilon_{CC}} \qquad (1)$$

The values of the LJ parameters (ϵ,σ) for the gas-gas and carbon-carbon interactions are: He (10.2, 2.56), Ne (35.6,2.75), Ar (120,3.4), Kr (171,3.6), Xe (221,4.1) and C (28,3.4). The length of the SWCNTs is 2.4 nm. As shown in Fig. 1, a group of carbon atoms along the bottom edge of CNT are fixed while the target atom and its neighbors are located on the top side of the tube. The incident atom is placed right above the target atom at a distance of $2.5\sigma_{GC}$ which is the cut off distance for Lennard-Jones potential. The CNT temperature is set at 300K initially. Then in the collision process, NVE is used since the interaction time between incident and target atoms is less than 1 fs. The simulation time step used is 10^{-5} fs. The initial velocity of the incident atom and the chirality of CNT are varied in the simulations to obtain the bond-breaking energy. The time history of the kinetic and potential energy of the target atom and its first, second and third neighboring atoms (see Fig. 1) are obtained.

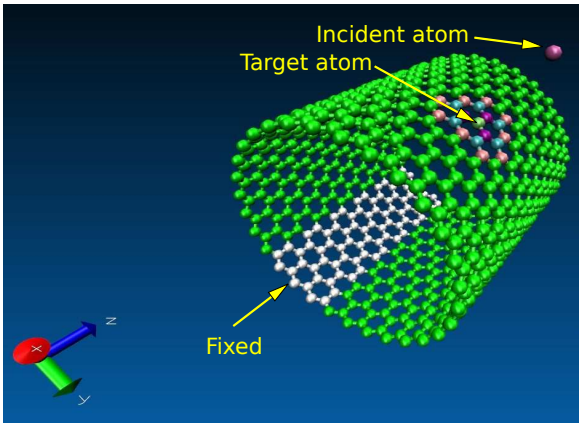

Figure 1: Dynamic response of a 2-D atom sheet.

Results and Discussion

Depending on the kinetic energy of the incident atom, three types collision behaviors are observed in our MD simulations: (1) the incident atom is reflected away from the CNT after collision without permanently dislocating the target carbon atom (denoted as R in Table 1); (2) the incident atom is reflected away after permanently dislocating (bond breaking) the target carbon atom (denoted as BR); and (3) the incident atom penetrates into the CNT after permanently dislocating the target carbon atom (denoted as BP). Table 1 shows the kinetic energy ranges of the incident noble gas atoms for these three collision behavior. For the lighter atoms (He and Ne), the minimum bond-breaking kinetic is nearly constant. The lightest atom, He, is always reflected back after the collision while Ne can penetrate into the CNT with a sufficiently high kinetic energy. For the heavier atoms (Ar, Kr, Xe) the minimum bond-breaking energy is proportional to their masses. Reflection is not observed in Xe-CNT collision. Xe atom always penetrates into the CNT after breaking the CNT bonds. Figure 2 shows that, while the minimum bond-breaking kinetic energy is different for different noble gas atoms, it is independent of the chirality (or diameter) of the CNT. Another collision characteristics is the energy loss of the incident atoms. As shown in Fig. 3, while the light atoms such as He (and H as reported in

[2]) lose a part of their kinetic energy after breaking the CNT bonds, the heavier atoms, Ar, Kr, and Xe, lose almost 100% of their kinetic energy after knocking out the target atom. The energy loss of the heavy atoms, which can not be explained by the classical binary collision theory, is due to the lower velocity of the heavy incident atoms as shown in Fig. 3. Figure 4 shows that, for the He-CNT collision, the neighboring atoms of the target atom do not absorb much of the impact energy due to the short He-C interaction time. However, the bond breaking in Ar-CNT collision case is different (shown in Fig. 5) where a significant energy wave propagates through the first, second, third neighbors and beyond, absorbing nearly all of the kinetic energy of the Ar atom.

Table 1: Incident kinetic energy (eV) ranges for reflection and bond breaking of CNT.

Element	R	BR	BP
Helium	KE<38	38<KE	NA
Neon	KE<38	38<KE<510	KE>510
Argon	KE<53	53<KE<175	KE>175
Krypton	KE<86	86<KE<112	KE>112
Xenon	KE<117	NA	KE>117

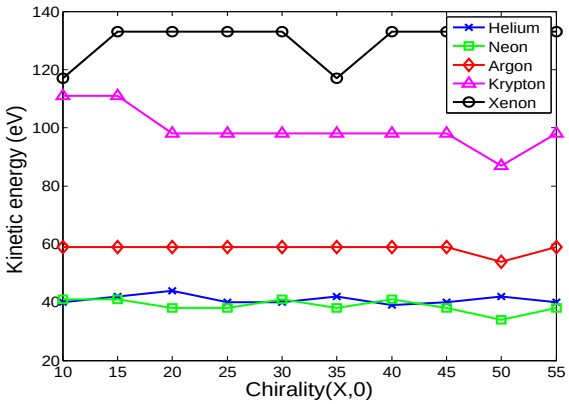

Figure 2: Minimum bond-breaking kinetic energy for SWCNTs with different chiralities .

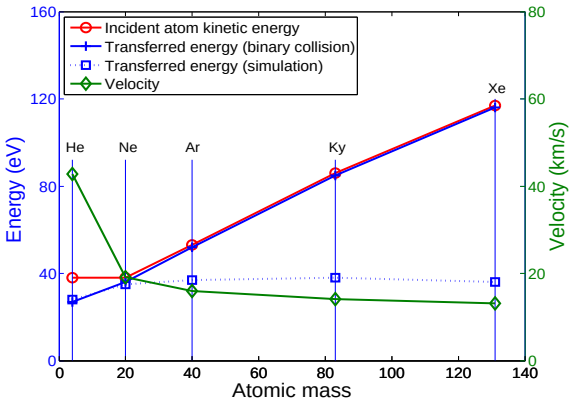

Figure 3: Energy transfer and velocity vs. atom mass.

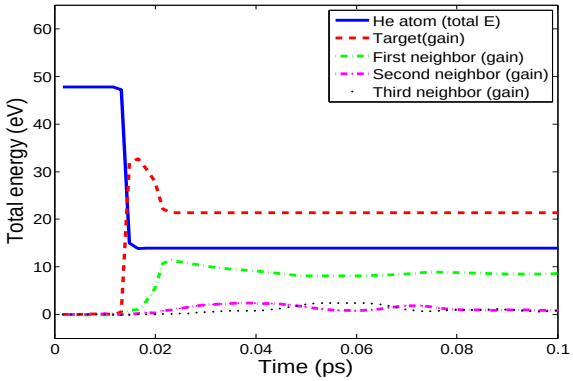

Figure 4: Energy exchange in He-SWCNT collision.

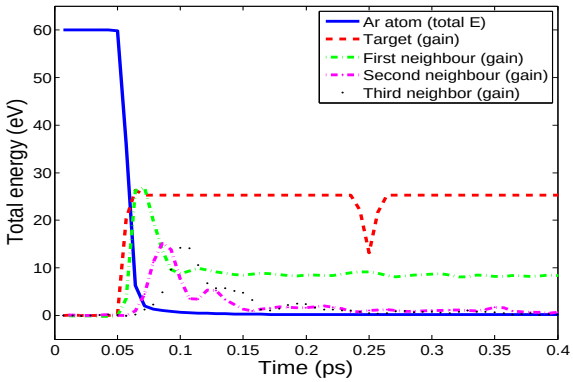

Figure 5: Energy exchange in Ar-SWCNT collision.

Conclusion

Collision of different noble gas atoms with single-walled carbon nanotubes exhibits different characteristics. It is observed that the minimum bond-breaking energy of the incident atom is independent of the chirality/diameter of the SWCNT. However, the incident atom mass plays an important role in the minimum bond-breaking energy, collision behavior and energy loss of the incident atom.

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