Molecular Dynamics Research of a Carbon Nanotube-buckyball Enabled Energy Attraction System

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Abstract An energy attraction system (EAS) composed of a carbon nanotube (CNT) with nested buckyballs is put forward for energy excess during impact owing to the outstanding mechanical attributes of both CNTs and buckyballs. Here we perform a series of molecular dynamics (MD) simulations to investigate the energy attraction capabilities of several different EASs based on a diversity of design parameters. For example, the effects of impact energy, the number of nested buckyballs, and of the size of the buckyballs are analyzed to optimize the energy attraction capability of the EASs by tuning the pertinent design parameters. Simulation results indicate that the energy attraction capability of the EAS is closely associated with the deformation characteristics of the confined buckyballs. A low impact energy leads to retrievable deformation of the buckyballs and the dissipated energy is mainly converted to thermal energy. However, a high impact energy yields non-retrievable deformation of buckyballs and thus the energy dissipation is dominated by the strain energy of the EAS. The simulation results also reveal that there exists an optimum value of the number of buckyballs for an EAS under a given impact energy. Larger buckyballs are able to disfigure to a larger degree yet also need less impact energy to induce plastic deformation, therefore performing with a better overall energy attraction ability. Overall, the EAS in this study shows a remarkably high energy attraction density of 2 kJ g⁻¹, it is a promising candidate for mitigating impact energy and sheds light on the research of buckyball filled CNTs for another applications.

Keywords: Carbon nanotube (CNT), buckyball, energy, Molecular dynamics (MD), effects, attraction.


1. Introduction

Energy attraction materials or structures have long been a hot research topic in engineering. [1,2] Their primary purpose is to protect critical structures or humans in a crash event by substantially mitigating the impact energy and loading magnitude. Traditionally, the maximum widespread material used for energy mitigation is metal due to its structural failure and plastic deformation. [3,4,5] Foam-filled columns [6-11] and sandwich structures [12-17] also show excellent implement in mitigating energy propagation due to their buckling mechanism. Another conventional form for energy attraction is internal damping by polymer composites. [18-22] However, these materials with an ultimate energy attraction density not exceeding 10 J g⁻¹ cannot satisfy the ever increasing requirement for lighter weight, smaller volume, and higher energy dissipation yield. [23] For example, polymer based nano-composite is superior to conventional polymer composite mainly because of its enhanced stiffness.27 A nanoporous energy attraction system consisting of non-wetting liquid and nano-porous particles possesses an energy attraction density about 15 J g⁻¹ larger than that of conventional systems. [23,27,28,29,30] CNT- based nano-composites also have properties which are conducive to energy attraction. [31-36] Carbon fiber reinforced plastic laminate, which is usually brittle, demonstrates good impact situation and absorbs a certain amount of impact energy when a coating of CNT-epoxy nano-composites is applied. [31] Further-more, the increasing understanding of the fullerene family [37,38,39] assists in designing novel energy attraction systems with much higher energy attraction density than those currently available. As a member of the fullerene family, carbon nanotubes (CNTs) have demonstrated excellent energy attraction capability in foams and three-dimensional sponge-array architectures [40,41,42] due to their unprecedented mechanical properties. Both experimental and computational results have revealed that CNTs have an extremely large surface area, high strength and stiffness, and are extraordinarily light weight compared to traditional materials, with a Young’s modulus of over 1 TPa, tensile strength of 200
GPa, shear modulus of about 1 GPa, bulk modulus of 462-546 GPa and bending strength of around 14.2 GPa [43,44,45]. Buckyballs, another important fullerene, are also verified to have intriguing mechanical confidants (bulk modulus of 903 GPa for an individual C6046) but alone deformation characteristics.48 Smith and Man [49,50] verified that C60 fullerene remained entire in low-energy collisions with graphite surfaces still had a large deformation in higher-energy collisions and this deformation was observed to rebound to the original configuration. Zhang and Becton [51,52] also investigated the phenomenon of buckyball-graphene collisions and found that the buckyballs bounced back under low impact energy still hold to the graphene and even penetrated through a single-layer of graphene at high impact energy with retrievable deformation. Xu et al. [53] found that for smaller buckyballs, impact energy was mainly converted to thermal energy, whereas larger buckyballs tended to have non retrievable deformation and thus strain energy was responsible for a majority of the energy dissipation, which was more beneficial for energy attraction systems. In addition, some experimental results reveal that core-filled CNTs, such as C60-Fe- and ZnS-filled CNTs, have much more enhanced mechanical confidants than empty CNTs. [54-58] However, few studies have focused on taking the benefits of structure strength from CNTs and the energy attraction capability from buckyballs. Therefore, this paper puts forward an energy attraction system made of buckyball-filled CNTs. The major functions of CNTs are structural support for carrying the mechanical load, maintaining the structural integrity, confining the buckyballs and reducing the contact force. Molecular dynamics (MD) simulations are carried out to investigate the impact performance and energy attraction capability of this EAS. To better understand the energy attraction characteristics, the effects of impact energy, the number of nested buckyballs, and the buckyball size on energy attraction performance are analyzed in addition to the progress of the deformation process during the impact procedure. This study can provide in-depth understanding of the impact confidants of buckyball-filled CNTs and offer a promising candidate for energy mitigation.

2. Model and Computational Methods

A single-walled carbon nanotube (SWCNT), a C180 buckyball, and a C720 buckyball [59,60,61] are selected to construct the energy attraction system (EAS) of interest. Figure 1 describe the computational model, in which the EAS is supported by a lower fixed rigid plate (receiver), and experiences an impact induced by the upper rigid plate (impactor) with a mass of 5.20 ng and a set of incipient impact velocities. According to the interlayer spacing (3.4 Å) of multi-walled carbon nanotube and the diameters of the C18 and C720 buckyballs, the diameter of the SWCNT in this study is chosen to be 31.8 Å. [62] For the EAS with five C720 fullerenes (5-C720 EAS), the distance L0 between the center of mass of two contiguous balls is set to be 28.4 Å and the length of the L SWCNT is 142 Å. For the purpose of simplification in terms of interatomic potentials, here we take both that, in terms of the number of carbon atoms, the impactor is the same length as the SWCNT and has a width equal to half of the environment of the SWCNT.

Therefore, throughout the whole system only carbon-carbon atomic interactions exist. In order to investigate the effects of the number of buckyballs on energy attraction performance, a set of different numbers of C720 buckyballs (2, 3, 4 and 5) are used to fill the SWCNT. To demonstrate the effect of buckyball size, twenty C180 buckyballs are used to make a 20-C180 EAS which has the same mass as the 5-C720 EAS.

In this work, MD simulations are carried out based on the open source platform LAMMPS (Large-scale Atomic/Molecule Massively Parallel Simulator). [63] In the incipient equilibrium process, a canonical ensemble (NVT) is applied to drive the temperature of the system to the desired 300 °K. Afterwards a micro canonical ensemble (NVE) is adopted in order to maintain the sum energy of the system. Therefore, the kinetic energy of the impactor is transferred and dissipated in the form of the potential and kinetic energy of the EAS. A pairwise 6-12 Lennard Jones potential is added to account for buckyball-buckyball and buckyball-CNT interactions.

\[
E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad r < r_c
\]

Where \(\varepsilon\) is the carbon-carbon potential well depth, \(\sigma\) is the critical distance where the carbon-carbon potential is zero, \(r\) is the distance between carbon atoms, and \(r_c\) is the cutoff. Here the value of parameters \(\varepsilon\) and \(\sigma\) are 2.875 meV and 3.47 Å respectively. [64,65] as well as, an optimal choice for carbon and hydrogen systems, the adaptive intermolecular reactive empirical bond orde (AIREBO) potential proposed by Stuart et al. [66] is utilized to demonstrate the carbon-carbon interaction intra-buckyball and intra-CNT including three terms as follows:

\[
E = \frac{1}{2} \sum_{i,j} \sum_{k \neq l} \left[ E_{ij}^{REBO} + E_{ij}^{12} + \sum_{k \neq i,l} E_{kj}^{TORSION} \right]
\]

Where \(E_{ij}^{REBO}\) the REBO (reactive empirical bond order) potential is developed by Brenner et al. [67] and demonstrates carbon-carbon interactions between atom i and j over a distance of less than 2 Å. The \(E_{ij}^{12}\) term, with an analogous form to the standard Lennard-Jones potential but excluding what the \(E_{ij}^{REBO}\) term includes, portray the longer-range pairwise interactions. Meanwhile a cutoff distance was set so as to control the extension of interactions captured by the \(E_{ij}^{REBO}\) term. As a tradeoff of computational efficiency and accuracy, the cutoff distance is determined as 10.2 Å in the willing work. Periodic boundary conditions are applied along the z-axis to prevent boundary effects and two standard 6-12 L-J walls are added to both sides of the SWCNT at \(x = \pm 26\) Å to restrict the SWCNT drifting excessively along the x-axis but reserving enough space for deformation during the impact process.
3. Results and Discussion

3.1. Effects of Impact Energy

To understand the effect of impact energy on the energy attraction capability of EAS, different impact velocities varying from 20 m s\(^{-1}\) to 400 m s\(^{-1}\) are applied to the impactor so as to generate different impact energies (from 64.88 eV to 10.138 keV) based on the 5-C720 EAS. All simulations demonstrate an important phenomenon wherein the deformation of both the SWCNT and the buckyballs exhibit different characteristics. For the SWCNT, during the impact process, a trapezoid deformation and an inverted trapezoid deformation alternatively evolve in turn. When the impact energy is very low, the deformation of the SWCNT is fully retrievable. For high impact energy, although the SWCNT cannot rebound to the original configuration absolutely, the non-retrievable deformation compared with buckyballs is negligible as demonstrated in Figure 2. For the buckyballs low impact energy also generates retrievable deformation. As the impact energy increases, non-retrievable deformation emerges in buckyballs gradually. Then all the buckyballs have non-retrievable deformation, and the evolution processes of their deformations are similar for a single impact. Afterwards the extent of non-retrievable deformation becomes more and more extreme until reaching a saturation state. The deformation of a buckyball can be illustrated to some extent by the radius of circulation (RoG) and the aspheric city value which are respectively expressed as:

\[
R_g = \left(\frac{1}{N} \sum_{i=1}^{N} (r_i - r_0)^2 \right)^{1/2} \quad (3)
\]

\[
b = \lambda_z^2 - \frac{1}{2} \left(\lambda_x^2 + \lambda_y^2\right) \quad (4)
\]

Where \(N\) is the number of carbon atoms in the buckyball, \(r_i\) and \(r_0\) are the positions of the \(i^{th}\) atom and the mass center of the buckyball respectively, \(\lambda_x, \lambda_y\) and \(\lambda_z\) are the principle moments of the circulation tensor.

Figure 2. Deformation evolution of the SWCNT with impact energy 4.152 keV. (a) The initial configuration of the SWCNT. (b) Its maximum deformation. (c) The final status after detachment among the impactor and the EAS. (d), (g) A loop of the trapezoid-shape deformation of the SWCNT during the process of (a) to (b) from the side view. (h) and (i) The deformation of the buckyballs when the detachment happens.
Figure 3 shows the evolution of the RoG and asphericity of a buckyball under two different impact energies 1.038 keV and 4.152 keV, representing two typical deformation mechanisms - fully retrievable and non-retrievable - respectively. Before the displacement of the impactor reaches 10 Å, the RoG of the buckyball hardly changes and little deformation of the buckyball become visible, as interactions between the impactor and buckyballs are very small. Before the impactor starts to rebound in the low impact energy case, the evolution pathway of the RoG for both cases almost coincide with each other since the impactors can reach the same distance for both cases. From the observation of the cross-section of crumpled buckyballs, it is noticed that a biconcave shape first become visible, and tends to become flatter as the impact continues, and then develops to a W-shape, during which the radius of circulation of this buckyball keeps reducing. However, when rebound happens in the low energy case the evolution pathways of the RoG in both cases deviates from each other, and the final morphology of the buckyball depends on the incipient impact energy. For the case of low impact energy, the deformation of the buckyball is reversible, and the evolution of the RoG reverses the pathway back to its original status. But in the case of high impact energy, the impactor continues to compress the EAS until the buckyballs become a “disk”, which results in a quick linear increase of the radius of circulation of the buckyball till the maximum value is quickly reached. As the impactor starts to rebound, the RoG of the buckyball experiences a quick drop to the value of 11.3 Å, and the morphology of the buckyball evolves to an intriguing V-shape. This V-shape then becomes unsymmetrical, resulting in the slight rise of the RoG of the buckyball. In what follows, the morphology as well as the RoG of the buckyball reaches a stable state, even though the deformation of the SWCNT continues to reverse until the impactor completely detaches from the SWCNT (see in Figure 2(h) and Figure 2(i)). Similar to the RoG, before the impactor starts to rebound in the low impact energy case, the evolution pathways of the asphericity for both cases almost coincide with each other since the impactors can reach the same distance for both cases. The difference is that the asphericity value keeps increasing generally with slight fluctuations during the
entire compression process. As the impactor starts to rebound, the asphericity experiences a short fluctuation and then reaches the summit at a V-shape. Afterwards it keeps decreasing until the detachment between the impactor and system happens. It is found that the asphericity during the rebounding process is always larger than that during the compression process while at the same displacement, due to the unretrievable deformation of the buckyball. Owing to the large deformation of the EAS, it is obvious that contact force among the impactor and receiver can be attenuated to a great extent compared with a rigid impact system. [68] Following the work-kinetic energy relationship, we can have

\[ \int F \cdot dy = \Delta E_k \]

Where \( F \) the contact force is induced on the impactor, \( y \) is the displacement of the impactor, and \( \Delta E_k \) is the difference value between the incipient impact energy (\( E_{\text{impactor}} \)) and the remaining kinetic energy (\( E'_{\text{impactor}} \)) after detachment of the impactor from the receiver. As depicted in Figure 4, the contact force shows a slow increase since the buckyball experiences a linear deformation at its early stage of impact and has enough room to hold the deformation. Then follows a short period of decrease in which the morphology of the buckyball experiences a transition change from a sphere to a biconcave structure leading to the reduction of interactions between the SWCNT, buckyballs and the impactor. After the short decrease, the contact force once again increases accompanied with a slight increase of the slope till the formation of a perfect biconcave structure. Once the W-shaped cross-section of the buckyball become visible, the rise of the contact force becomes quicker since the deformation of the buckyball is close to its limit and it becomes more and more difficult to densify the buckyball. When the compression ends, the contact force arrives at the summit value.

During the rebound process, the contact force drops rapidly to a value close to zero and then approaches zero steadily because the unretrievable deformation of buckyballs increases the interaction distance and further reduces the interaction between impactor and the remaining part of system. The area surrounded by the closed curve in the contact force-displacement plot indicates the work done by the contact force which has been confirmed to be equal to the energy attracted by the EAS. With the growth of impact energy, the impactor deforms the EAS further accompanied by an increase in the maximum contact force and an increase in the energy attraction by the EAS.

In order to quantify the relationship between the energy attraction efficiency of the EAS and impact energy, here we define the energy attraction efficiency \( \eta \) as \( \Delta E_{\text{impactor}} / E_{\text{impactor}} \).

According to the principle of conversation of energy, it can be expected that the energy absorbed by the EAS is partially converted to increased kinetic energy of atoms in the EAS (\( \Delta E_{\text{kinetic}} \)) and the remaining part is transformed to its extra potential energy (\( \Delta E_{\text{potential}} \)). Since the kinetic energy of all the atoms (\( E_{\text{kinetic}} \)), the center-of-mass kinetic energy of the EAS (\( E_{\text{m,kinetic}} \)) and the thermal energy (\( E_{\text{thermal}} \)) can be respectively expressed as:

\[
E_{\text{kinetic}} = \sum_{i=1}^{N} \frac{1}{2} m_i v_i^2 ,
\]

\[
E_{\text{m,kinetic}} = \frac{1}{2} M \vec{v}^2
\]

and

\[
E_{\text{thermal}} = \sum_{i=1}^{N} \frac{1}{2} m_i (v_i - \vec{v})^2
\]

Where \( m_i \) is the mass of the \( i^{th} \) atom, \( v_i \) is the velocity of the \( i^{th} \) atom, \( M \) is the mass of the EAS and \( \vec{v} \) is the center-of-mass velocity of the EAS, we can get their relationship as follows:

\[ E_{\text{kinetic}} = E_{\text{m,kinetic}} + E_{\text{thermal}} \]  \hspace{1cm} (6)

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Figure 4. Contact force as a function of impactor displacement during the impact process with various impact energies as velocity increases from 80 m/s-1 to 160 m/s-1
Figure 5. Increased thermal energy and center-of-mass kinetic energy as well as the temperature of the EAS under impact energy 4.152 keV, as a function of time

Figure 6. Energy attraction rate and maximum contact force upon impact with various impact energies (from $6.488 \times 10^{-2}$ keV to 10.138 keV)

Figure 5 describes the evolution process of the two parts and the temperature of the EAS under an impact energy of 4.152 keV, which indicates that the major part of $\Delta E_{\text{kinetic}}$ accounts for the excessive thermal energy causing the increase of the temperature while the rest of it is responsible for the moderate movement of buckyballs and SWCNT. The increment of the potential energy $\Delta E_{\text{potential}}$ is mainly comprised of the strain energy of EAS caused by deformation while the rest of it is attributed to the relative motion between fullerenes. To better determine the dominant factor of the energy attraction and identify the roles $\Delta E_{\text{kinetic}}$ and $\Delta E_{\text{potential}}$ play during the impact process, we classify the impact behavior into two phases as shown in Figure 6. In phase I, it can be observed that most of the absorbed energy during the impact is transferred to the increase of the kinetic energy of the EAS indicating that the absorbed kinetic energy plays a dominant role in energy attraction in phase I. In detail, the energy attraction rate rises sharply from 15.49% to 40.37% at point A ($E_{\text{impact}} = 0.406$ keV) as the impact energy grows. However, after reaching the relative summit value, the rate decreases to 28.19% at point B ($E_{\text{impact}} = 1.622$ keV). Meanwhile, the difference between the absorbed kinetic energy and potential energy gradually decreases and is almost zero at point B. Point A where both the
absorbed potential and kinetic energy by the EAS reaches a relative summit value is considered to be the point of the best energy attraction in phase I. The explanation of the characteristics in phase I can be elaborated as follows: the deformation of the buckyballs in this stage is retrievable after the impactor detaches from the EAS and thus the variation of the potential energy of the system is relatively small.

Meanwhile, the constraint placed on the positions of fullerenes by the L-J walls poses an obstacle for the EAS to dissipate more energy from the impact via the increase of the kinetic energy of fullerenes. With respect to phase II, the energy attraction rate rises again due to the rapid increase of the absorbed potential energy and the slow increase of the absorbed kinetic energy of EAS after point B. This is because the non-retrievable (plastic) deformation of a number of buckyballs become visible gradually and thus absorbs the impact energy in the form of the increased strain energy. It is interesting to point out that all buckyballs exhibit non-retrievable deformation after point C (E_{impactor} = 2.741 keV) where the energy attraction rate is similar to that at point A still with different proportions of energy transformation. At point D (E_{impactor} = 4.688 keV), the energy attraction rate achieves the maximum value (56.93%) and the difference between the two converted energies also reaches a summit, indicating that the absorbed energy due to the plastic deformation of buckyballs reaches its maximum value and the absorbed potential energy plays the dominant role in this stage. Therefore, after point D the energy attraction efficiency keeps reducing since the EAS reaches its limiting energy attraction capability. Figure 6 also reveals that as the impact energy increases the maximum contact force induced on the impactor keeps rising and the trend gets sharper at lower impact energies and lessened at higher impact energies.

### 3.2. Effects of the Number of Buckyballs

To better understand the effects of the number of buckyballs, comparisons of the CNT-buckyball system and pure CNT are discussed in terms of mechanical behavior and energy attraction capability. Lateral compression is performed for the mechanical behavior. The relationship of stress and strain for both systems is depicted in Figure 7. In the early stage of the stress-strain curve, the lateral compression Young’s modulus is estimated as 5 GPa for the CNT-buckyball system based on linear elastic theory. It is obvious that, compared to the pure CNT, the compressive capability of the CNT buckyball system is enhanced to a great extent. There also exist a few big summits in the stress-strain curve of the CNT-buckyball system, which corresponds to the morphological evolution of C720 (as the insertions in Figure 7). For comparison of energy attraction capability, both the CNT buckyball system and pure CNT had an impact energy of 4.15 keV applied. Then they are further compared with the pure buckyballs system, which was proven to have a favorable energy attraction capability in the previous work. [68] The comparison results are exhibited in Table 1. It can be noticed that the energy attraction efficiency of a single CNT is low and the contact force is much larger than that of the other two systems. This can be explained as the CNT is very flexible to deform in the lateral direction and therefore prone to become flattened during the impaction but most of its deformation is retrievable after the impactor detaches from it, which can be inferred from the contact force-displacement curve during the loading and unloading process in Figure 8. The comparison results also reveal that the buckyballs only system has an energy attraction efficiency 15.02% higher than the CNT-buckyball system. The reason is that buckyballs in the buckyballs only system possess more severely un retrievable deformation, which can be seen in the subplots of Figure 8. However, according to Table 1, the maximum contact force of the buckyballs only system is 49.25% larger than that of the CNT-buckyball system. Therefore, by taking into account the energy attraction capability and maximum impact force together, the CNT-buckyball system is considered to be a better EAS for impacts. In order to investigate the effect of the number of buckyballs on the EAS energy attraction capability, 5-C720 EAS, 2-C720, 3-C720 and 4-C720 EASs are used to perform the impact test. According to the stress-strain relationships of the four EASs depicted in Figure 9, it can be inferred that the EAS with more buckyballs possesses larger stiffness, that is to say, more impact energy is required to deform the buckyballs. Thus an EAS with more C720 balls needs more impact energy for the transition from the kinetic to potential dominated phase, which means for EASs with more than C720 balls, the impactor needs to do more work to arrive at the same displacement. Therefore the EAS can store more energy according to the work-energy theorem, resulting in a better energy capacity. For the purpose of comparison, impact simulations of different EASs are based on the same series of impact energy per unit mass (IEUM, defined as $E_{impactor}/m_{EAS}$, where $m_{EAS}$ is the mass of EAS) ranging from 0.04 kJ g-1 to 4.15 kJ g-1 between the systems. As has been discussed in Section 3.1, when the IEUM is very low, the deformation of the buckyballs is retrievable. Simulation results show that an EAS with more buckyballs needs a larger IEUM to produce the non-retrievable deformation in buckyballs.

That is, as the IEUM increases, non-retrievable deformation first become visible in 2-C720 EAS, followed by 3-C720 EAS and so on. The reason is maybe because the buckyballs’ mass comprises an increasing proportion of the total mass of the EAS. Figure 10 shows the energy attraction status with IEUMs of 1.30 kJ g-1 and 3.32 kJ g-1 respectively. In the case where the IEUM is 1.30 kJ g-1, only 2-C720 EAS has non-retrievable deformation and therefore it shows the largest energy attraction. For the rest of the EASs, the energy attraction increases slightly with the increase of the number of buckyballs. In the case with IEUM 3.32 kJ g-1, all the buckyballs of the different EASs have non-retrievable deformations, and as a result the energy attraction improves with the increase of the number of buckyballs. Furthermore, energy attraction per unit mass (EAUM) determined by $\Delta E_{impactor}/m_{EAS}$ is investigated. According to Figure 11, for a certain EAS, EAUM grows with the increasing IEUM. When IEUM increases from a small value wherein only retrievable deformation of buckyballs happens, the maximum EAUM is acquired first by 2-C720 EAS and then from 3-C720 EAS to 5-C720 EAS in order. It is obvious that there exists an optimal IEUM for an EAS to fulfil its energy
attraction capability and this value becomes larger with more buckyballs. When the IEUM reaches 0.66 kJ g\(^{-1}\), non-retrievable deformation occurs in 2-C720 EAS and thus the corresponding EAUM becomes larger than those of the other EASs. As the growth of IEUM continues, more extreme deformation improves the energy attraction capability. Therefore, when non-retrievable deformation of 3-C720 EAS occurs to a certain degree, its EAUM exceeds that of the 2-C720 EAS. As seen in Figure 11, the maximum EAUM moves rightwards from IEUM =0.66 kJ g\(^{-1}\) to IEUM = 2.66 kJ g\(^{-1}\) where 5-C720 EAS obtains the optimal EAUM. As the impact energy increases, the deformation of the EAS reaches its limit from the 2-C720 EAS to the 5-C720 EAS in order.

Figure 7. Stress-strain curves for both CNT/buckyballs and CNT only systems under lateral compression

Table 1. Comparisons of the three energy attraction systems

<table>
<thead>
<tr>
<th></th>
<th>CNT/buckyballs</th>
<th>Buckyballs</th>
<th>CNT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy absorption efficiency</td>
<td>56.34%</td>
<td>64.8%</td>
<td>9.79%</td>
</tr>
<tr>
<td>Maximum contact force (μN)</td>
<td>1.734</td>
<td>2.588</td>
<td>6.91</td>
</tr>
</tbody>
</table>

Figure 8. Contact force-displacement relationship during the loading and unloading process of the impact.
Figure 9. Stress-strain curves for 2-C720, 3-C720, 4-C720, 5-C720 EASs and 20-C180 EAS under lateral compression.

Figure 10. Energy attraction (including potential energy and kinetic energy) of 2-C720, 3-C720, 4-C720 and 5-C720 EASs with IEUM = 3.32 kJ g⁻¹ and 3.32 kJ g⁻¹ respectively.

Figure 11. A fitting surface of EAUM of C720 EAS as a function of number of buckyballs and IEUM based on cubic spline interpolation. Number of buckyballs varies from 2 to 5 and IEUM varies from 0.05 kJ g⁻¹ to 5.19 kJ g⁻¹.
Upon the impact with the same IEUM, the EAS shows a lower EAUM than the others when it reaches the deformation limit first. However, after all EASs reach their deformation limit, an EAS with more buckyballs presents a larger EAUM. To design a high-performance impactor receiver, besides the energy attraction per unit mass, the energy attraction efficiency, which also can be calculated from EAUM/IEUM, is another important criterion for evaluating the capability of energy attraction systems. Here we perform a series of simulations on the C720 EASs with the IEUM from 1.30 kJ g\(^{-1}\) to 5.19 kJ g\(^{-1}\) such that the non-retrievable deformation happens at least in one of the four C720 EAS. As Figure 12 shows, at IEUM=1.30kJg\(^{-1}\), the energy attraction rate of 2-C720 EAS is much larger than those of other EASs because only 2-C720 EAS shows the non-retrievable deformation in the 2-C720 buckyballs. The energy attraction rate of 3-C720 EAS increases greatly with the IEUM from 1.30 kJ g\(^{-1}\) to 1.87 kJ g\(^{-1}\) but is still less than that of 2-C720 EAS. It can be explained that the non-retrievable deformation just occurs in the 3-C720 EAS but the 2-C720 EAS evolves into a deeper buckling morphology.

![Figure 12](image1.png)

**Figure 12.** Energy attraction percentage of C720 EAS as a function of number of buckyballs, based on a series of IEUMs (varying from 1.30 kJ g\(^{-1}\) to 5.09 kJ g\(^{-1}\)).

![Figure 13](image2.png)

**Figure 13.** Energy attraction percentage of 2-C720, 3-C720, 4-C720 and 5-C720 EASs respectively as a function of IEUM (varying from 0.05 kJ g\(^{-1}\) to 5.09 kJ g\(^{-1}\)).
The highest energy attraction rates at IEUM = 2.54 kJ g⁻¹ and IEUM = 3.32 kJ g⁻¹ are obtained by the 4-C720 EAS and 5-C720 EAS respectively because of their significant non-retrievable deformations. With the increase of impact energy the energy attraction rate of the EAS decreases after the EAS achieves its deformation limit as we have discussed in Figure 13. EASs with fewer buckyballs arrive at the first summit more quickly and have a larger summit value of energy attraction percentage in phase I because there is more space in the SWCNT for buckyballs moving to absorb impact energy and transfer it into kinetic energy. Besides that, EASs with fewer buckyballs enter into phase II earlier due to the larger stiffness and then achieve the second summit faster as well, yet have a lower summit value. That is because buckyballs as the major energy dissipation part are a relative small proportion of the total mass in the EAS. Moreover, since the EAS with fewer buckyballs is easier to reach its deformation limit and then have less EAUM, it can be inferred that the energy attraction efficiency of EASs with fewer buckyballs becomes steady more quickly and has a larger final rate. Consequently, it is essential to choose the appropriate number of buckyballs for an EAS to optimize its energy attraction performance.

3.3. Effects of Buckyball Size

Since the 5-C720 EAS and 20-C180 EAS have the same mass, the same impact energy means the same IEUM. According to Figure 9, it is also indicated that a tiny force is required to deform the 20-C180 EAS when the strain is less than 0.35. The reason is that at the beginning the buckyballs randomly arrange in the tube because of an equilibrium process and then position themselves almost in a plane following impact causing the CNT to become flatter (which can be seen in Figure 14(a) and (b)). During this process, little deformation become visible in C180 balls. Hereafter the stiffness of 20-C180 EAS becomes significantly large and soon surpasses that of 5-C720 EAS. Impact velocities varying from 20 m s⁻¹ to 200 m s⁻¹ are given to the impactors of both the two EASs. The simulation results show that upon impact with enough energy C180 fullerenes in an EAS also exhibit non-retrievable deformation capability, although to a lesser extent than C720. Thus more storage energy in C180 balls will be transferred back to the impactor during the rebound process, resulting in less energy attraction. For example, Figure 14 shows the deformation evolution of C180 buckyballs during the impact process with an impact velocity of 160 m s⁻¹, which can be compared with the results in Figure 3. After the buckyballs position themselves in a plane, the deformation evolution, similar to that of the C720 buckyball but more simple, experiences biconcave, disk and biconvex shapes in order. As a result, the two EASs show a similar changing pattern of energy attraction capability with the increase of impact energy irrespective of their own characteristics. As is shown in Figure 15, the energy attraction increases with the increase of impact velocity and the absorbed potential energy takes up a large portion of the absorbed total energy until the EAS reaches its deformation limit. At the incipient stage, the increase of the energy attraction by EAS is gentle followed a quick increase, when the non-retrievable deformation occurs in the EAS, towards a saturated status because of the deformation limit.

3.3. Effects of Buckyball Size

Since the 5-C720 EAS and 20-C180 EAS have the same mass, the same impact energy means the same IEUM. According to Figure 9, it is also indicated that a tiny force is required to deform the 20-C180 EAS when the strain is less than 0.35. The reason is that at the beginning the buckyballs randomly arrange in the tube because of an equilibrium process and then position themselves almost in a plane following impact causing the CNT to become flatter (which can be seen in Figure 14(a) and (b)). During this process, little deformation become visible in C180 balls. Hereafter the stiffness of 20-C180 EAS becomes significantly large and soon surpasses that of 5-C720 EAS. Impact velocities varying from 20 m s⁻¹ to 200 m s⁻¹ are given to the impactors of both the two EASs. The simulation results show that upon impact with enough energy C180 fullerenes in an EAS also exhibit non-retrievable deformation capability, although to a lesser extent than C720. Thus more storage energy in C180 balls will be transferred back to the impactor during the rebound process, resulting in less energy attraction. For example, Figure 14 shows the deformation evolution of C180 buckyballs during the impact process with an impact velocity of 160 m s⁻¹, which can be compared with the results in Figure 3. After the buckyballs position themselves in a plane, the deformation evolution, similar to that of the C720 buckyball but more simple, experiences biconcave, disk and biconvex shapes in order. As a result, the two EASs show a similar changing pattern of energy attraction capability with the increase of impact energy irrespective of their own characteristics. As is shown in Figure 15, the energy attraction increases with the increase of impact velocity and the absorbed potential energy takes up a large portion of the absorbed total energy until the EAS reaches its deformation limit. At the incipient stage, the increase of the energy attraction by EAS is gentle followed a quick increase, when the non-retrievable deformation occurs in the EAS, towards a saturated status because of the deformation limit.

Figure 14. Deformation evolution of C180 buckyballs of a 20-C180 EAS with impact velocity 160 m s⁻¹
What is different is that non-retrievable deformations of the 20-C180 EAS and 5-C720 EAS occur at impact velocities of at least 100 m s\(^{-1}\) and 120 respectively, which means that the C180-EAS needs a higher impact energy for non-retrievable deformation because of the larger stiffness. At the instant of impact (with an impact velocity of 20 m s\(^{-1}\)) the energy attraction of the C180 EAS is much larger than that of C720 EAS. Because the impact energy is so low it makes little influence on the C720 EAS but it is also able to flatten the SWCNT during the compression process and thus place the disordered buckyballs in a plane. Then when the impact velocity rises to 40 m s\(^{-1}\), the energy attraction of the C720 EAS climbs fast, however, this impact energy has little further influence on the C180 EAS and thus the increase of the energy attraction is relatively small. Afterwards, the energy attraction of the C180 EAS also enters into an ascending stage following that of the C720 EAS, which is also reflected in Figure 16. Likewise, the C180 EAS experiences similar phases \(I\) and \(II\) as we have discussed for the C720 EAS in Section 3.1. Compared with the C720 EAS, the transition for the C180 EAS happens at a high impact energy due to its larger stiffness. Since C180 can hold a relatively small deformation compared to C720, the C180 EAS absorbs less impact energy and leads to a smaller energy attraction percentage. In addition, the maximum contact force keeps rising with impact velocity from 20 m s\(^{-1}\) to 200 m s\(^{-1}\) for both the two EASs with a growing increment speed. The force exerted on the 20-C180 EAS is higher than that on the 5-C720 EAS for a
variety of impact velocities. Generally, the 5-C720 EAS possesses a better energy attraction performance than the 20-C180 EAS, as it bestows a larger energy attraction rate but a smaller contact force.

4. Conclusions

In this paper, an EAS consisting of a CNT and multiple nested buckyballs is put forward, and its energy attraction capability is investigated by performing a variety of MD simulations of impacts with different design parameters including impact energy, the number of nested buckyballs and the size of those buckyballs. Effects of these parameters are analyzed in detail in order to determine the best energy attraction capability of the EAS. Simulation results state that the deformation characteristics of the confined buckyballs play a crucial role in the energy attraction capability of the EAS. At low impact energy buckyballs exhibit retrievable deformation and thus the energy attraction mainly owes to the increased thermal energy. At high impact energy buckyballs present non-retrievable deformation and the mitigated energy is mainly converted to strain energy of the EAS, which is more beneficial for energy attraction ability. An EAS with larger stiffness needs more impact energy for the transition from the kinetic to potential energy dominated phase. The results also indicate that under certain impact energies the EAS can improve its energy attraction ability by tuning the number of nested buckyballs. It is also found that larger buckyballs perform a better energy attraction capability because they generate larger deformation at the same impact energy and need a lower impact energy to yield plastic deformation. In addition, this EAS reveals a remarkable high energy attraction density, as much as 2 kJ g\(^{-1}\), which is especially available for weight-controlled products requiring the capability of crash worthiness such as an aircraft. Overall, although this research is performed in silicon, the results can provide a promising candidate from a computational viewpoint for impact protection and energy dissipation, and offer insights into the research of buckyball-filled CNTs in other fields. Future work should be devoted to expand the realm of the impact energy the EAS can hold and further improve the energy attraction capability of the EAS, for example, the effects of the size of the SWCNT, comparison of the SWCNT and MWCNT (multi-walled carbon nanotube), and the effects of the rolled layers of the MWCNT. Since plenty of free space between SWCNT and buckyballs exists, fluids or gases such as water and CO\(_2\) can be placed to investigate their effects on energy attraction capability of EASs. Previous research\(^{28,29,70}\) has provided compelling evidence that the change of solid-liquid or solid-gas interaction energy can be part of energy dissipation, thereby enhancing the system’s energy attraction.

References


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