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# Ballistic resistance capacity of carbon nanotubes

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**Abstract**
Carbon nanotubes have high strength, light weight and excellent energy absorption capacity and therefore have great potential applications in making antiballistic materials. By examining the ballistic impact and bouncing-back processes on carbon nanotubes, this investigation shows that nanotubes with large radii withstand higher bullet speeds and the ballistic resistance is the highest when the bullet hits the centre of the CNT; the ballistic resistance of CNTs will remain the same on subsequent bullet strikes if the impact is after a small time interval.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Diverse applications of carbon nanotubes (CNTs) have been envisioned due to their remarkable chemical, mechanical, electronic and magnetic properties [1]. They are being considered to make useful articles such as artificial muscles, reinforced materials, bulletproof vests, explosion-proof blankets, etc. In the past, various types of materials such as wooden and metal shields were used as body armour to protect humans from injury in combat. With the invention of firearms, they became ineffective. New ballistic-resistant body armour has been developed using, for instance, multiple layers of Kevlar, Twaron and Dyneema fibres [2]. When a bullet strikes body armour, the fibres of these materials absorb and disperse the impact energy to successive layers to prevent the bullet from penetrating. However, the dissipating forces can still cause non-penetrating injuries which is known as blunt force trauma. Even when the bullet is stopped by the fabric, the impact and the resulting trauma would leave a severe bruise and, at worst, damage critical organs. Hence the best material for body armour should have a high level of elastic storage energy that will cause the bullet to bounce off or be deflected.

The energy absorption capacity of different radii CNTs under ballistic impact has been reported in two extreme cases in which the bullet moved with constant speed [3]. For a nanotube with one end fixed, the maximum load bearing bullet speed of the nanotube increases and the energy absorption efficiency decreases with the increase in relative heights at which the bullet strikes; these values have been found to be independent of the nanotube radii when the bullet hits at a particular relative height. For a nanotube with both ends fixed, the energy absorption efficiency reaches the minimum when the bullet hits around a relative height of 0.5. The challenge in exploring the ballistic resistance capacity of carbon nanotubes lies in the understanding of the bullet impact mechanism involving how the force, energy, momentum and velocity vary in the time domain at ballistic striking. The present research aims to resolve this problem.

## 2. Computational methodology

Single-walled carbon nanotubes (27, 0), (22, 0) and (18, 0) of radii 10.576 Å, 8.608 Å and 7.051 Å having a length, $L$, of about 75 Åwere used in this investigation. The nanotubes were fixed at both ends to represent roughly its condition within a composite. A piece of diamond ($35.6 \times 35.6 \times 7.1$ Å$^3$) was used as a bullet, with its tip width being several orders of magnitude larger than that of a flattened nanotube. This, in a sense, mimics the real situation since the width of a real bullet is always larger than that of the biggest nanotube after flattening. The bullet was released from a position about 15 Å from the centre axis of the nanotube at different heights, $h$, with a speed varying between 1000 and 3500 m s$^{-1}$, as shown in figure 1. The initial bullet speeds for which the nanotubes could bear without any bond breakage or detachment were

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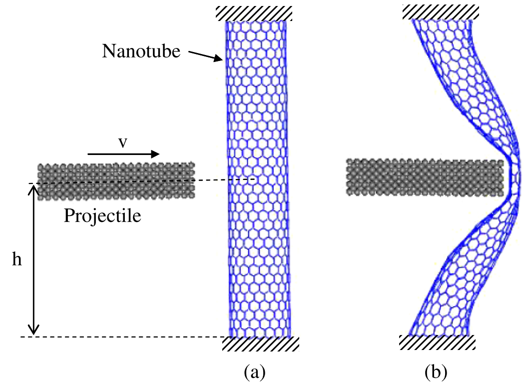


**Figure 1.** The molecular dynamics model of a carbon nanotube subjected to ballistic impact. (a) Initial model, (b) a deformed (18, 0) nanotube at its maximum energy absorption.

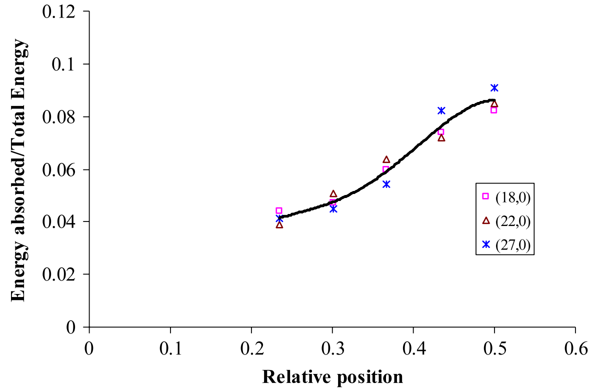


**Figure 2.** Variation of relative absorption energy with the relative positions ($\rho$) of the nanotubes at which the bullet strikes.

estimated from the maximum absorption energy of the CNT that was determined in a separate simulation by shooting the bullet with an arbitrarily selected constant speed of 400 m $s^{-1}$. A range of values, around this estimated speed, were used as the initial speeds of the bullet and, since its release, the speed was recalculated after every time step of 0.5 fs using the principle of energy conservation, i.e. after every time step, the kinetic energy of the bullet was calculated by subtracting the energy absorbed by the nanotube in the previous time step, assuming there was no other energy loss. Hence, to avoid the heat dissipation, only two rows of atoms that are next to the fixed rows of atoms at each ends were taken as thermostat atoms. As the impact deformation takes place in a very short duration, the heat dissipation via the thermostat atoms at the ends of the CNT would be minimal. The ballistic performance of a nanotube was examined using the classical molecular dynamics analysis for bullets released at various positions with speeds that would only elastically deform the nanotubes.

In this work the atomic interactions within the nanotube were described by a three-body Tersoff–Brenner potential [4, 5] that has been used to simulate various deformation processes [6–10] of carbon nanotubes. The non-bonded interaction between the bullet and nanotube were described by a two-body Morse potential, $V(r_{ij}) = D[e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}]$, which has been successfully used for a large number of machining and indentation processes involving substrate–tool interactions [11–13]. The parameters used in the Morse potential are: $\alpha = 5.110$ Å$^{-1}$, $D = 139.71$ kcal mol$^{-1}$ and $r_0 = 2.522$ Å.

## 3. Results and discussion

### *3.1. Understanding the dynamic properties*

A bullet moving with a constant speed towards a nanotube that is fixed at both its ends will deform the nanotube which absorbs the energy of the bullet. Eventually, the nanotube will be broken regardless of the magnitude of the bullet speed. Thus the energy difference of the CNT before its interaction with the bullet and just before the onset of fracture gives the maximum absorption energy of the CNT. In reality, from the moment of impact, the speed of a bullet would begin to decrease as it hits any object and eventually either the bullet would bounce back as the speed became zero or the bullet would penetrate the object if the initial speed is high enough. Thus the initial bullet speed for a bouncing-back process is estimated by equating the maximum absorption energy of the nanotube as calculated above to the kinetic energy of the bullet, i.e.

$$E_{\text{abs}} = E_f - E_i = \tfrac{1}{2} m V_{\text{ini}}^2, \qquad (1)$$

where $E_f$ is the energy of the nanotube just before breakage and $E_i$ is that before the CNT–bullet interaction, $m$ is the mass of the bullet and $V_{\text{ini}}$ is the initial bullet velocity. In our simulation, the decrease of the bullet speed at every time step is determined by the law of energy conservation, i.e. by equating the energy absorbed by the nanotube to the decrease in kinetic energy of the bullet. The bullet is then bounced back as the nanotube releases its energy elastically stored and $V_{\text{bb}}$ is determined when the bullet bounces off the CNT and attains a constant value.

It was found that the highest bullet speed which a nanotube can bear is a function of the nanotube radius, $R$, and the relative impinging location of a bullet on the nanotube defined by $\rho \equiv h/L$, where $L$ is the length of the nanotube and $h$ is the distance between the bullet impinging point and an end of the nanotube as shown in figure 1(a). A bigger tube, as it can absorb more energy, withstands a greater bullet speed, $V_{\text{ini}}$ and the energy absorbed increases as $\rho$ increases and reaches its maximum at $\rho = 0.5$. However, as shown in figure 2, the variation of relative absorption energy with $\rho$ (i.e. the maximum energy absorbed normalized by the total energy of the nanotube before impact) or the variation of energy absorbed per unit area with $\rho$ is very similar when $R$ changes, showing that these quantities are not really dependent on the nanotube radius. On the other hand, the maximum absorption energy varies almost linearly with nanotube length, as shown in figure 3.

Figure 4 shows the variation of the bullet speed with time $t$ during its impacting–bouncing process when the bullet struck at different positions on a (18, 0) nanotube. This shows that the bullet started to bounce back almost at the same time irrespective of its initial speed and the position of striking. However, the deceleration and the acceleration of the bullet are different. This is because the nanotube deformation depends on $\rho$. The variation of bullet speed (curve 1), bullet–nanotube

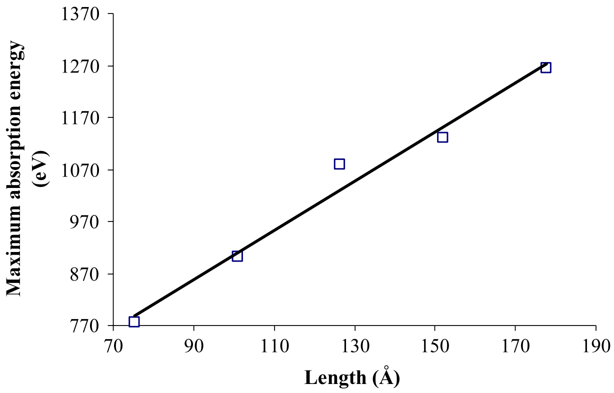


**Figure 3.** Variation of the maximum energy absorbed with nanotube length.

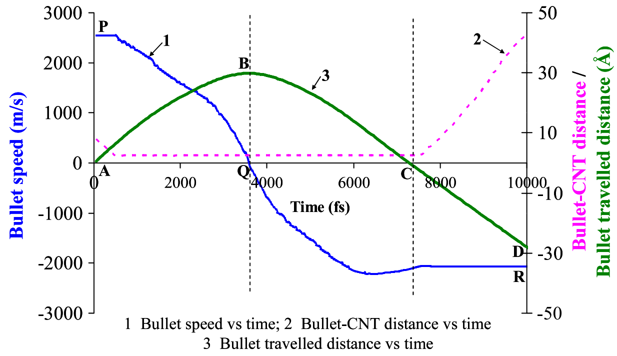


**Figure 5.** Variation of different properties of a bullet with time during its impact and bouncing-back processes when impacting the middle of a (18, 0) nanotube.

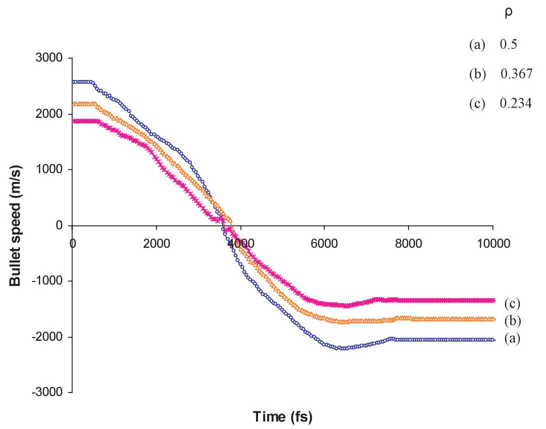


**Figure 4.** Variation of the bullet speed with time during its impact and bouncing-back processes. Note also the variation with the bullet impact location, $\rho$. The nanotube used for this analysis is an (18, 0) nanotube.

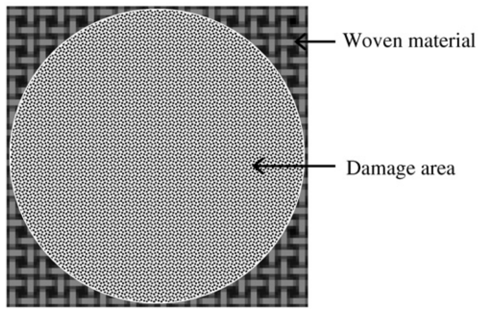


**Figure 6.** A schematic showing a layer of woven carbon nanotube yarn material.

distance (curve 2) and the bullet travelling distance (curve 3) with time are shown in figure 5 when the bullet impacts at the centre of a (18, 0) CNT. Part PQ of curve 1 represents the speed variation during the impact and part QR of the curve stands for that during the bouncing back. We can see that the bullet attains a constant bouncing-back speed $V_{bb}$ when $t = 7850$ fs, which is lower compared to the initial impact speed of the bullet $V_{ini}$, indicating that a certain amount of energy is retained by the nanotube when the bullet bounces off. The impact process is represented by AB in curve 3. When the bullet speed becomes zero at point B, it starts to bounce back. Thus BCD represents the bouncing-back process. At C ($t = 7300$ fs) the bullet has returned to its initial impact position, but curve 2 shows clearly that it is still in contact with the nanotube. The bullet departs from the nanotube at a much later time, $t = 7850$ fs, due to the reverse elastic deformation of the nanotube in releasing its stored energy.

If a subsequent impact takes place immediately after the first bullet's bouncing off, the nanotube cannot withstand the same speed although its microstructure was not damaged under the first impact. For instance, for an (18, 0) nanotube, the maximum load bearing speed and the maximum absorption energy on the second impact are 2200 m s$^{-1}$ and 572.8 eV, compared to 2560 m s$^{-1}$ and 775.6 eV, respectively, for the first impact. This is because immediately after the first impact, the nanotube has not completely released the elastic energy retained from the first impact which reduces its capacity for absorbing further energy. On the third impact these values become 2050 m s$^{-1}$ and 497.3 eV, respectively. However, the above changes do not influence the bouncing-back speed of the bullet.

If a subsequent ballistic impact occurs not immediately after the first, e.g. only after 12.5 ps, the nanotube's performance remains the same, because this short duration is long enough to allow full release of the elastic energy stored in the nanotube. This means that nanotubes have an excellent resistance to repeated ballistic impacts, which is essential for body armour and explosion-proof blankets.

### *3.2. A case study*

Based on the properties of CNTs obtained above, we can carry out a case study as a potential application example. We may very roughly estimate the thickness of a possible CNT body armour material composed of several layers of woven carbon nanotube yarns illustrated schematically in figure 6, if we can assume that the above nanoscale property can be extended simply to a macroscale case. One may argue that, as in the mechanical property characterization of metals, a nanoscale property cannot be extended to the macroscopic scale directly because of the scale-effect. This is true because a metal is a single crystal on the nanoscale, but possesses a polycrystalline structure on the macroscale which contains numerous grain boundaries and makes the metal significantly weaker compared with its single-crystalline state. However, the situation with a CNT is rather different. When a CNT is grown, its diameter is in nanometres but its atomic structure along its length, in micrometres, does not change. In other words, it is completely different to the metal case of the microstructural change from monocrystalline to polycrystalline. Hence, as a first approximation, it is reasonable to make the above assumption because the length change of CNTs does not involve atomic structure change.

Baughman [14] has demonstrated that carbon nanotube fibres can be easily woven into textiles. Carbon nanotube yarns of various diameters (3.2–100 $\mu$m) have been made by spinning [15–17] and the carbon nanotubes in a yarn will have much better mechanical strength than loose individuals [18]. Let us take yarns of diameter 100 $\mu$m and, for simplicity, assume that a yarn is only a bundle of loose carbon nanotubes. Such a yarn can have about $5 \times 10^9$ (18, 0) nanotubes of 14.1 Å in diameter. Supposing this yarn is used to make potential armour material, the thickness of the material that may protect the wearer from a revolver bullet can be estimated as follows. According to John Schaefer [19], a popular police revolver bullet of 0.358 inches (9.1 mm) in diameter would damage an area of 0.101 inch$^2$ (0.652 cm$^2$). Hence, to cover this area, about 180 nanotube yarns of about 0.9 cm in length will be needed to form a woven fabric. Since the maximum absorption energy is approximately a linear function of the nanotube length, as discussed before, a single nanotube yarn of the above dimension will absorb 0.344 J. Thus the nanotubes in the impact area will absorb 62 J/layer. To prevent damage to the wearer, the body armour in the impact area should be able to elastically absorb all the muzzle energy of the bullet [20], 320 J. This means that six layers of woven nanotube yarn material are sufficient. If the thickness of a layer equals the diameter of a yarn, the thickness of the body armour material to absorb all the muzzle energy of the bullet will be 600 $\mu$m.

## 4. Conclusion

This study shows that the ballistic resistance capacity of a carbon nanotube is highest when the bullet hits its centre and a larger tube withstands a higher bullet speed. On a subsequent impact after a small time interval, a nanotube could withstand almost the same speed as in the first impact, indicating that carbon nanotube body armour can have a constant ballistic resistance even when bullets strike at the same spot. This study estimates, though based on a very strong assumption, that body armour of 600 $\mu$m in thickness made from six layers of 100 $\mu$m carbon nanotube yarns could bounce off a bullet with a muzzle energy of 320 J.

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