Energy absorption capacity of carbon nanotubes under ballistic impact

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Carbon nanotubes have great potential applications in making ballistic-resistance materials. This letter analyzes the impact of a bullet on nanotubes of different radii in two extreme cases. For a nanotube with one end fixed, the maximum nanotube enduring bullet speed increases and the energy absorption efficiency decreases with the increase in relative heights at which the bullet strikes; these values are 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 minimum when the bullet strikes around a relative height of 0.5. © *2006 American Institute of Physics*.
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The remarkable mechanical, electrical, and thermal properties of individual carbon nanotubes (CNTs) have been known for some time.[1] In addition CNTs have very high aspect ratio. This combination of properties makes them as an ideal candidate for reinforcing polymers and actual components in rectifiers, nanoswitches, and sensors.[2] Material heterogeneity, impurities, and difficulty in uniform dispersion due to their aggregation into bundles have hindered their realization in several applications. Scientists have been working hard on making use of these nanotubes to make useful articles that exploit these properties.

Some other potential applications include making artificial muscles, bullet-proof vests as light as a T-shirt, shields, and explosion proof blankets. For these applications, thinner, lighter, and flexible materials with superior dynamic mechanical properties are preferred. Especially in making bullet-proof vests, shields, and explosion proof blankets, the best material will have a high level of elastic storage energy that will cause the projectile to bounce off or be deflected, i.e., the objective is to reduce the effects of "blunt trauma" on the wearer after being struck by a bullet. However, very little is known on the resistance and energy absorbing capacity of CNTs under high velocity impacts. Currently, the Kevlar fiber having a toughness of ~33 J/g m (Ref. 3) is widely used in bullet-proof vests. When a bullet strikes body armor, these fibers absorb and disperse the impact energy that is transmitted to the vest from the bullet, causing the bullet to deform. The speed of rifle bullets varies between 180 and 1500 m/s.[4,5] For example, cartridges having primer in rim send bullets at 370–460 m/s and cartridges having primer in the center propel bullets at a much faster rate of 740–920 m/s; the Swift cartridges drive its bullet at over 1220 m/s. The bullet's traveling speed depends on its size, shape, and the air density.

In this work, we investigate the relationship between the nanotube radius, the relative position at which the bullet strikes, the bullet speed, and the energy absorbed by the nanotube for a particular bullet size and shape.

Single-walled CNTs (27,0), (18,0), and (9,0) of radii 10.576, 7.051, and 3.525 Å, respectively, all having a length of ~75 Å, were used in this investigation. Two extreme cases, where the nanotubes fixed (i) at one end to a rigid surface and (ii) at both ends, were examined. A piece of diamond having 1903 atoms with dimensions of $35.67 \times 35.67 \times 7.13$ Å^3 was used as a bullet with its speed varying from 100 to 1500 m/s. The bullet dimension was selected such that the width is larger than the width of the biggest nanotube after flattening. The bullet was released from a target about 15 Å from the center axis of the nanotube and moved at a constant speed in the horizontal direction (i.e., perpendicular to the nanotube axis), as shown in Figs. 1(a) and 1(b). The nanotube performance was examined for bullet released with various speeds at various positions using the classical molecular dynamics (MD) method.

In the MD method the atomic interactions were described by a three-body Tersoff-Brenner potential,[6,7] which has been used to simulate various deformation processes of CNT. As pointed out in our earlier work[8] on nanotubes, in order to minimize the heat conduction problem and improve the computational efficiency, Berendsen thermostat was applied to all atoms except those rigidly held. At the beginning the energy of the CNTs was relaxed and minimized by the conjugate gradient method. In a typical process, when the bullet strikes the object, the speed would decrease. However, in this study we make the bullet travels horizontally at a constant speed to avoid unnecessary complications and study the energy absorption behavior of the nanotube by calculating its energy at certain time intervals.

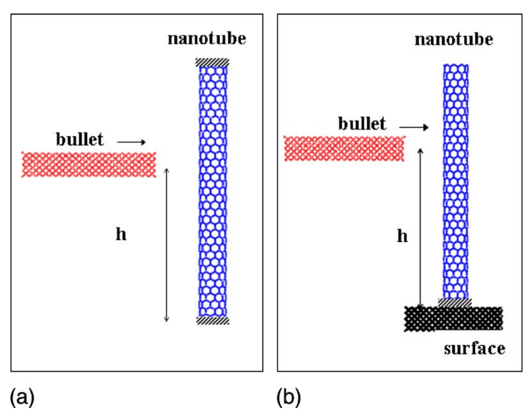

FIG. 1. (Color online) Initial models for MD simulation (a) with both ends fixed and (b) with one end fixed (only a portion of the rigid surface is shown for convenience).

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TABLE I. Maximum absorption energy of three different radii nanotubes when the bullet strikes the nanotube at various relative heights.

	(9,0) tube of radius 3.53 Å			(18,0) tube of radius 7.05 Å			(27,0) tube of radius 10.6 Å		
	One end fixed		Both ends fixed	One end fixed		Both ends fixed	One end fixed		Both ends fixed
h/L (ρ)	Speed (m/s)	E_{abs} (eV)	E_{abs} (eV)	Speed (m/s)	E_{abs} (eV)	E_{abs} (eV)	Speed (m/s)	E_{abs} (eV)	E_{abs} (eV)
0.31	360	139.9	219.1	360	225.4	414.2	340	510.1	654.9
0.45	650	189.6	385.6	600	429.0	656.8	600	652.7	896.4
0.61	950	298.3	399.0	870	616.0	692.8	850	781.8	937.3
0.71	1080	291.2	307.7	1050	558.8	333.8	1050	752.7	525.1
0.85	1400	196.3	166.2	1400	363.1	139.1	1450	670.2	256.5

The relative height, ρ at which the bullet was released, the maximum absorption energies, and the corresponding bullet speed of the nanotubes with three different radii are given in Table I. In the case where one end of the nanotube is fixed, when the bullet struck the nanotube with higher speeds than those listed here either the bullet passed through the nanotube breaking it into two pieces or the nanotube detached at the fixed end.

In the case where the nanotube was fixed at both ends, bullet was released at a constant speed of 400 m/s. As the bullet struck, the nanotube was indented, flattened around that area, and bent, as shown in Figs. 2(a) and 3(a). Flattening and bending continued for some time and eventually either the nanotube was broken or detached at one end. During the shooting process the nanotube absorbed some energy. The energy absorbed increased with time, reached a maximum value, and then decreased due to breakage or detachment of the nanotube. At this moment the temperature of the nanotube also increased by about 20–30 K. However, this temperature change was very little to account for any thermal energy contribution. The maximum energy absorbed tabulated in Table I reached its maximum when ρ is around 0.5.

In the case where one end was fixed, as the bullet struck, the nanotube was indented; the stress developed was passed along the nanotube in both directions. When the bullet hits the nanotube at low ρ values, initially the stress was released by sagging and buckling near the base. (Hence, the bullet with high speed detached the nanotube at the base due to the dynamic effect.) Further stress developed caused the nanotube to flatten around where the bullet struck and bend near the buckle, as shown in Fig. 2(b). The flattening and bending continued until the bullet passes away. During this period the stress was released mainly via the top end of the nanotube. When the bullet hits the nanotube at high ρ values, initially the nanotube did not buckle near the base. This is because the stress developed was released via the top end. The upper portion of the nanotube bent a little and the nanotube flattened where the bullet struck, as shown in Fig. 3(b). Flattening and bending continued for some time. Then the nanotube buckled near the base and started to sag [Fig. 3(b)]. The speed of the bullet for which the nanotube could be resilient increased linearly with the relative height ρ [Fig. 4(a)]. At low ρ values, the bullet speed was low. As a result, the entire portion of the nanotube that was above the struck point bent and flattened over a period of time as the stress was developed and released at the same time. During this the absorption energy of the nanotube was almost constant. However, all these happened in 1/100 of a nanosecond. The maximum bullet speed for which the nanotube could be resilient is almost independent of its radii when the bullet struck a nanotube at a particular ρ value. The maximum absorption energy of the nanotube was higher when the bullet struck the nanotube at about 62% of its length [Fig. 4(b)]. When the bullet struck the nanotube above $\rho > 0.62$, the temperature of the nanotube also increased by about 100–200 K. This means that some energy is converted into thermal energy. However, we find that the thermal energy kT (where k is the Boltzmann constant) is only about 0.01% of the calculated absorbed energy.

Energy absorption behavior is often characterized by the absorption efficiency ε, which can be defined as

$$\varepsilon = \frac{W}{F_{\max} L},$$

where W is the absorbed energy at a given deflection L and $F_{\max}$ is the maximum load received by the nanotube up to this deflection. Accordingly when one end of the nanotube was fixed, the calculated ε values for all three nanotubes at $\rho=0.45$ is about 0.2 and at $\rho=0.61$ is about 0.1. Thus, although the absorption energy of the nanotube increases with

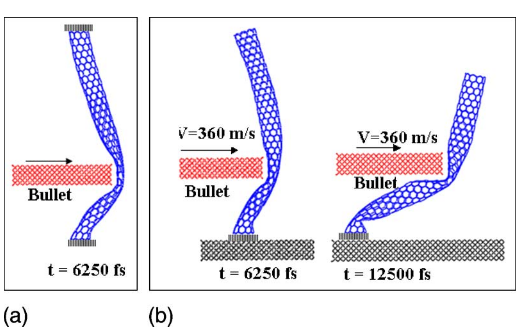


FIG. 2. (Color online) Bullet strikes the (9,0) nanotube at a relative height of 0.31 (a) with both ends fixed and (b) with one end fixed.

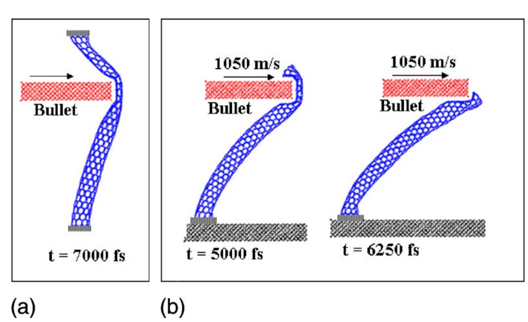
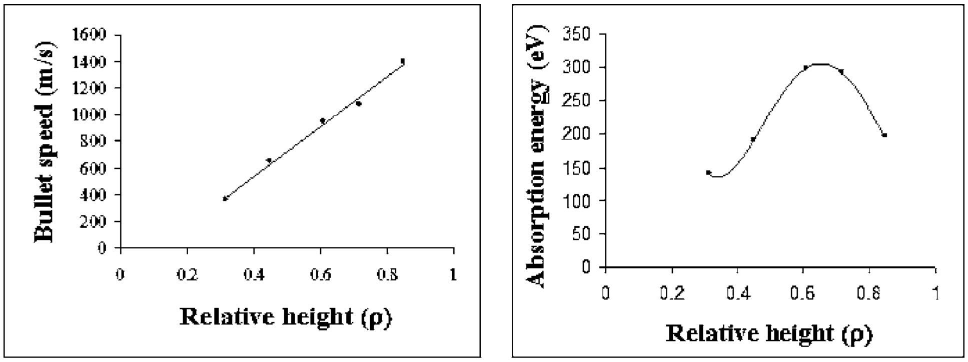


FIG. 3. (Color online) Bullet strikes the (9,0) nanotube at a relative height of 0.71 (a) with both ends fixed and (b) with one end fixed.



(a) (b)

FIG. 4. Variation of (a) nanotube enduring bullet speed and (b) maximum absorption energy with the relative height at which the bullet strikes a (9,0) nanotube fixed at one end.

radius, the calculated absorption efficiency at a particular ρ value is independent of its radius. However, for a nanotube, ε decreases as ρ increases. This could be due to the higher nanotube enduring bullet speed at higher ρ values—where there was not enough time for the nanotube to absorb. On the other hand, for a nanotube fixed at both ends, ε is minimum around $\rho=0.5$.

In summary, for a nanotube with one end fixed, our study shows that carbon nanotubes could be resilient to projectile traveling at speeds of 200–1400 m/s; the nanotube enduring projectile speed increases whereas the absorption efficiency decreases with the increase in relative height ρ. For a nanotube with both ends fixed, the absorption energy reaches maximum whereas the absorption efficiency reaches minimum when the bullet strikes the nanotube in the middle.

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