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Highly effective energy dissipation system based on one-dimensionally arrayed short single-walled carbon nanotubes

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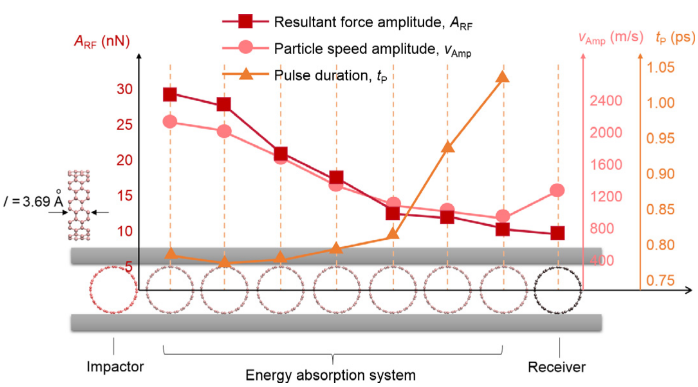
GRAPHICAL ABSTRACT



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ABSTRACT

In this paper, the impact energy dissipation characteristics of one-dimensional (1D) short single-walled carbon nanotube (SWNT) system are investigated via molecular dynamics (MD) simulation. It is found that 1D SWNT system has good force mitigation performance and extraordinarily high specific energy absorption (SEA) upon high-speed impact in the absence of plasticity, which is 1 to 2 orders advantageous over macroscale impact protection devices and structures. Moreover, a simple model based on the theorem of momentum can give an accurate prediction of force mitigation effect. The mechanism of this non-plastic impact energy dissipation lies in the transformation of impact energy to the kinetic and potential energy of SWNT molecules. Similar to macroscopic metallic rings, SWNTs can buckle under large force, which in fact enhances force mitigation capability of the system. A continuum model is established, able to predict the critical forces of SWNTs of different radii. Finally, system performance upon impact speeds in a broader range and the influence of parameters such as system length and SWNT radius are discussed. This work may be instructive to the design of novel impact energy mitigation system at nanoscale.

1. Introduction

Substantial damages are caused by impact incidents from time to time, e.g. road traffic accidents, earthquakes and projectile attacks. Various types of energy mitigation devices and structures

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are designed such as hydraulic shock absorbers in vehicular suspension [1] and honeycomb structures [2] widely used in aeronautics and astronautics industry. However, there are intrinsic failings in traditional macroscale impact protections, one of which is relatively low specific energy absorption. Especially, traditional impact energy absorptions exhibit extremely heavy reliance on plastic deformations [3] which disables the reusability. It is of critical importance to find possible solutions to above problems.

One of the alternatives is to be "small". It is commonly recognized that downsizing can contribute to the enhancement of strength and ductility to a great extent. Resorting to nanoscale, carbon nanotubes (CNTs), thanks to their extraordinary mechanical properties such as ultra-high specific strength and specific modulus [4], have been attracting considerable attention [5–7]. They also exhibit remarkable flexibility and resilience upon large deformation [8]. It has been shown that various forms of CNT arrays, for example, vertically aligned CNT bundles, can have a good energy dissipation capability due to sequential buckling [9–11] whose mechanical properties can be further improved by carbon ion irradiation [12]. It is thus reasonable to view CNTs as a promising candidate for efficient and reusable energy dissipation purpose.

2. Simulation descriptions

2.1. Simulation method

In this paper, the energy dissipation characteristics of 1D SWNT system is studied via MD simulation, which may be regarded as a counterpart of widely studied 1D metallic ring system in impact engineering [13]. The whole simulated system contains 9 short (length $l = 3.69$ Å) (16,16) SWNTs with their symmetry axes parallel, as is described in Fig. 1(A). The distance between adjacent SWNTs is 24.873 Å [14], which is the equilibrium spacing of two SWNT molecules. The energy dissipation system is composed of 7 SWNTs in the middle of the 9-SWNT chain and the SWNTs at two ends serve as the impactor (with an initial speed $v_{\mathrm{Imp}} = 3500$ m/s) and the receiver respectively. To maintain the one-dimensionality of the system, the SWNT chain is tightly held by an ideal frictionless rigid lateral wall.

The detailed information on MD simulations is given as follows. Simulations are conducted based on LAMMPS (large-scale atomic/molecular massively parallel simulator) platform [15] and are visualized by VMD (visual molecular dynamics) [16] program. Full atomistic description of SWNTs is applied. The carbon–carbon (C–C) interaction of intra-SWNT is modeled by the adaptive intermolecular reactive empirical bond order (AIREBO) potential, as has been widely used to simulate graphene, CNT and buckyball system [17,18], while C–C interaction of inter-SWNT is accounted for by an Lennard-Jones (L-J) model $U(r) = 4\varepsilon\left[(\sigma/r)^{12} - (\sigma/r)^{6}\right]$ for the van der Waals interaction, where U is the L-J potential for two atoms; r is the distance between atoms; ε and σ are two L-J parameters, representing the depth of the potential well and the finite distance for zero the inter-particle potential respectively, which are chosen as $\varepsilon = 0.086$ kcal/mol and $\sigma = 3.400$ Å [19]. The time integration step is 1 fs. The system is first run for equilibrium in NVT ensemble (the canonical ensemble) at $T = 10$ K for 10 000 fs to achieve a low thermal vibration level about equilibrium positions, followed by a 7000 fs simulation in NVE ensemble (the micro-canonical ensemble) for stress wave propagation through the system. Resultant force history on each SWNT is recorded. The constraint of ideal wall is achieved by zeroing lateral resultant force.

2.2. Simulation results

Simulation results are presented in Fig. 1(A), showing that as stress wave propagates through the 1D SWNT system, both resultant force amplitude (representing wave amplitude) and particle speed amplitude decrease and pulse duration on single SWNT increases (which could be explained by energy conversion and will be discussed later). This is intrinsically different from 1D buckyball system studied in our previous work, where solitary wave is supported [20]. Phenomenal dissipation performances such as significant force ratio η (defined as $\eta = A_{\mathrm{Rec}}/A_{\mathrm{Imp}}$, where A_{Imp} and A_{Rec} are amplitudes of impact force on 1D SWNT system and force on the receiver respectively) and ultra-high specific energy absorption (SEA) are observed: $\eta = 0.278$ and SEA $= 760.0$ J/g, which is almost 1–2 orders of magnitude larger than its counterpart in macroscale. The total energy absorption is 84.84 eV, which is 86.9% of the initial kinetic energy of the impactor. The instantaneous temperature of 1st SWNT of the dissipation system is kept below the temperature causing thermal instability of CNT [21]. Furthermore, no plastic behavior is observed during the impact process, while the thermal vibration level of SWNTs increases after being passed through by stress wave.

3. Model for force mitigation

A simple model is developed to quantitatively depict the force mitigation effect of the system. Assuming that stress wave speed is unchanged during propagation within single SWNT, the time durations from perfect ring shape to maximum deformation and from maximum deformation to perfect ring shape are both one-half of pulse duration on single SWNT. Because the impactor, energy dissipation system and the receiver are composed of identical SWNTs, the speed of impactor should drop to zero after impact and the speed of receiver should rise from zero, which are both confirmed by simulation. Thus, using the theorem of momentum, we have

$$\begin{aligned} -mv_{\mathrm{Amp},0} &= -F_{0,1}\frac{t_{\mathrm{P},1}}{2} \\ mv_{\mathrm{Amp},i} &= \left(F_{i-1,\,i} - F_{i,\,i+1}\right)\frac{t_{\mathrm{P},i}}{2}, \quad 1 \le i \le N-1 \\ mu_{\mathrm{Amp},N} &= F_{N-1,\,N}\frac{t_{\mathrm{P},N-1}}{2} \end{aligned} \tag{1}$$

where m is the mass of SWNT. $v_{\mathrm{Amp},i}$ and $t_{\mathrm{P},i}$ are particle speed amplitude and pulse duration on ith SWNT (0th represents the impactor SWNT) respectively. $F_{i,i+1}$ is the average interaction force between ith and $i+1$th SWNTs. Suppose force amplitude on a SWNT is proportional to the average force, from Eq. (1), we may further have

$$\eta = \frac{A_{\mathrm{Rec}}}{A_{\mathrm{Imp}}} = \frac{F_{0,1}}{F_{N-1,\,N}} = \frac{v_{\mathrm{Amp},0}t_{\mathrm{P},N-1}}{v_{\mathrm{Amp},N}t_{\mathrm{P},1}} \tag{2}$$

and

$$\frac{A_{i-1,\,i} - A_{i,\,i+1}}{A_{i,\,i+1} - A_{i+1,\,i+2}} = \frac{v_{\mathrm{Amp},i}t_{\mathrm{P},i+1}}{v_{\mathrm{Amp},i+1}t_{\mathrm{P},i}}, \quad 1 \le i \le N-2 \tag{3}$$

where $A_{i,i+1}$ is the force amplitude between ith and $i+1$th SWNTs. Eq. (2) relates the system force mitigation effect (force ratio η) to particle speed amplitude and pulse duration and Eq. (3) predicts force reduction in a recursive manner. These relations are tested in Fig. 1(B), which illustrate that for various types of SWNT and system lengths, this model can describe the force mitigation effect very well.

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