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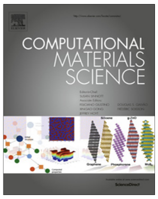

Atomistic-scale simulations of mechanical behavior of suspended single-walled carbon nanotube bundles under nanoprojectile impact

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ABSTRACT

Carbon nanotube fiber (CNTF) is generally considered a strong candidate for the fabrication of bullet-resistant vests due to its excellent combination of extremely high elastic modulus, high yield strain, low density, super toughness, as well as good flexibility. CNTF may also provide effective dissipation of impact energy through fibrillation within the CNTF and through disintegration of the CNTF. In this study, molecular dynamic (MD) simulations are performed to investigate the nanoprojectile impact on suspended single-walled carbon nanotube (SWCNT) bundles. The simulated results show that the fronts of impact-induced longitudinal and transverse waves travel at speeds ranging from 18 to 20 km/s and 1.5 to 1.7 km/s in the bundles that absorb most of the nanoprojectile's initial kinetic energy. The manner in which ballistic impact energy spreads within the CNTF is predicted to be mainly through transverse waves. Acoustic vibrations of the SWCNT bundle caused by the impact-induced longitudinal and transverse waves are revealed. We propose that impact energy can be effectively dampened in a manner of generating acoustic noise and heat. The threshold of the nanoprojectile's incidental kinetic energy is calculated and is used to evaluate the breaking of SWCNT bundle. The destructive role of a lap joint within the SWCNT bundle is demonstrated, as well as the role of local buckling in blocking the propagation of transverse and longitudinal waves. To facilitate the spreading of impact energy over a long distance, we propose that polymers may form an ideal matrix that should be infiltrated in the CNTF through capillary forces to increase the impact strength and to reinforce the wave spreading to release.

1. Introduction

Desirable features for bullet-resistant vests are that they be lightweight, air-permeable and soft. These features make bullet-resistant vests more comfortable to wear and more applicable in various occasions and circumstances. Inspired by these requirements, today's generation of soft bullet-resistant vests are developed using tightly woven layers, such as woven Kevlar and Dyneema fibers, to protect the wearer from gun bullets and stab attacks [1,2]. When a bullet strikes fiber-textile body armor, the tightly woven layers of fiber textile can diffuse its impact through spreading impact-induced plane and shear waves over a large portion of the vest to resist the ballistic impact. The kinetic energy of the projectile is absorbed by the fiber textile, allowing the projectile to be stopped before it penetrates into the inner layer of the textile. To reduce blunt trauma injuries to wearers after being struck by a bullet or stabbed, the best fiber should have a high level of strain energy storage. Specifically, these fiber textiles are required to absorb and disperse the ballistic impact energy that is transmitted to the textile and then causes fiber fibrillation, fiber elongation, breakage, and disintegration of fabric structure [1,2]. Carbon nanotube fiber (CNTF) is an ideal alternative fiber due to its excellent combinations of extremely high elastic modulus, high yield strain, low density, good toughness and flexibility [3–6]. Therefore, CNTF presents enormous potentials for the fabrication of thinner, lighter and flexible bullet-resistant vests [5,7].

Several methods, including wet spinning [8], CVD forest spinning [9,10], CVD aerogel spinning [11], and electro-spinning [12], have been reported to produce the "super" CNTF characterized as raw carbon nanotubes (CNTs) with a large aspect ratio that has been spun into yarn-like textiles. Especially in densified dry-spun CNTF, CNTs are bundled into many sub-bundles and stacked to obtain both good CNT alignment and superior CNT volume fraction.

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The tensile properties of dry-spun CNTF are now comparable to those reported for top fibers [13].

It is worth noting that a bullet's impact energy can be additionally dissipated through the CNT fibrillation within CNTF and through the disintegration of the yarn-like structure of the CNTF. It is most likely that, under ballistic impact, CNTF would result in a great number of interface interactions between CNTs. Since each CNTF has a very large interface area per unit volume and is composed of billions of CNTs (Fig. 1), the CNTF promises greater absorption of ballistic energy than other solid fibers.

The basic components of CNTF are CNT bundles, within which CNTs adhere to each other through van der Waals attraction. The two-dimensional hexagonal structure of sp2-bonded carbon atoms forms the basis of graphene and CNT. Molecular dynamic (MD) simulations have shown that longitudinal and transverse waves travel at speeds of about 20 km/s and 3.4 km/s respectively on monolayer graphene [14,15]. Thus, we expect that CNT bundles might also be able to spread waves at high speeds that are beneficial to the diffusion of balletic impact. Two situations are often encountered for CNTs within CNTF. One occurs when CNTs lap with each other to form long bundles within the CNTF, resulting in many gaps between these lap-joint CNT bundles. The other is the presence of local buckling in CNTs, usually introduced during spinning densification of CNTF. The influences of lap-joint bundles and local buckling on the propagation of impact-induced waves have not yet been clarified. If lap joints and local buckling slow or block the spreading of impact energy through blocking the passage of longitudinal and transverse waves, then the efficiency of impact diffusion would be jeopardized. This would result in early failure of the CNTF textile at the instant of impact as the energy absorption capacity is exceeded. Therefore, detailed analyses are significant in gauging the capacity of the energy absorption and diffusion of the CNTF. Research in this aspect is beneficial to the design and modification of the manufacture of CNTF for bullet-resistant uses [16,17].

In bullet-resistant applications, efficient diffusion of a bullet's impact over a wide area requires the propagation of both longitudinal and transverse waves through CNT bundles. Because the flexibility of CNTF is an important feature for the transport of transverse waves along CNT bundles, in comparison with multilayer CNTs, CNTF made from single-walled CNTs (SWCNTs) characterized by lower bending rigidity due to their smaller diameter is more suitable for the fabrication of bullet-resistant vests. In-depth understanding of the impact resistance of SWCNT bundles should enhance this fabrication process.

MD simulation represents an elementary brick of a through-process modeling approach that has wide applications in study of the mechanical properties of graphene and CNTs [14,15,18–23]. Various mechanical properties of carbon nanotubes were evaluated using MD simulations [24–27]. The main subjects in these studies were analyzing the influences of different processing conditions, such as tensioning [24], rotating nanotubes in uniform liquid argon flow [25], water interaction [26], compression [27] on the mechanical properties. However, it should be noted that mechanical behavior of carbon nanotubes in response to external impact still needs to be investigated. It would be useful to understand the impact resistance of carbon nanotubes while interacting with a high-speed project. Hence, in the present study, MD simulations are performed with the maximum allowed bond-force criterion to investigate impact tests of a high-speed nanoprojectile on suspended SWCNT bundles. Impacts are inflicted on SWCNT bundles of three types: continuous, lap jointed, and featuring local buckling. The formation and propagation of the impact-induced shock waves are simulated at the atomic scale. The effectiveness in absorption of a high-speed nanoprojectile's kinetic energy by SWCNT bundles of various thicknesses is analyzed. The thresholds of the initial kinetic energy of the high-speed nanoprojectile for determining the failure of SWCNT bundles are calculated. Through monitoring variation in the kinetic energy of SWCNT bundles after impact, the acoustic vibrations of SWCNT bundles during shock waves propagation are revealed. Acoustic vibrations of CNT bundles can generate acoustic noise and heat and should be an effective way of damping impact energy.

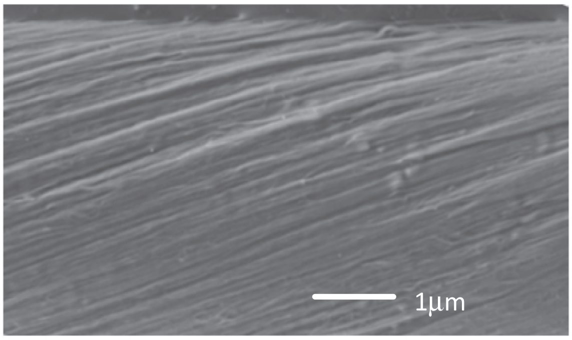

Fig. 1. Scanning electron microscopy image of dry-spun CNT fibers.

To reveal the influences of lap joint and local buckling on the spread of impact energy, two further simulations of impact bundles with lap joint and local buckling are conducted. We show that both a lap joint and local buckling can block the passage of shock wave energy and limit the capability of the CNTF to diffuse impact energy. Finally, we propose that polymers may be an ideal matrix for infiltration in CNTF via capillary forces to increase crosslinks between adjacent CNTs to reinforce wave spreading.

2. Methodology

For impact tests, a nanoscale cubic diamond (termed "n-bullet" in this study) is chosen as a projectile in order to minimize the impact-induced elastic deformation energy stored by the projectile, because diamond is known as the hardest material. The projectile is non-rigid. Normally, reactive force field simulations present plastic deformation of CNTs, characterized by the appearance and spreading of topological defects via bond breaking and reforming [28–30] that can theoretically occur at room temperature at very high strains (>20%). Scanning electron microscopy and transmission electron microscopy evidence shows that the fracture surfaces of broken CNTs are typically sharp and flat, indicating that CNTs break in a brittle manner at room temperature [23,31–34]. This means that the bond breakage and SWCNT breakage can be determined when a maximum allowed bond force is exceeded. The maximum allowed bond force is selected as 10 nN in the current study. Here, we use molecular dynamics (MD) with a maximum allowed bond force criterion to detect the bond breakage which evolves into a crack that propagates until complete failure. In this study, MD simulations are executed using the LAMMPS MD simulator [18] with the nonreactive COMPASS ('Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies') force field [22]. The COMPASS force field is widely used in commercial software Materials Studio and has been validated in simulating the variations in potential arising from small elastic deformations [35–37], thereby enabling accurate and simultaneous predictions of SWCNT structural deformation.

The tensile force on each atom is computed using a symmetric per-atom stress tensor [14,18,23]. Atomic-resolution color maps are constructed to depict force distribution throughout SWCNT bundles. Based on the characteristics of force fields, the amount of energy required to break a covalent carbon-carbon bond is