Mechanical Deformation of Carbon Nanothread Bundle

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Abstract

The superior toughness of carbon nanotube fibres makes them attractive for many applications in energy-related fields, such as mechanical energy storage and energy harvesting [1], artificial muscles, soft robotics [2], flexible electronics [3]. This work explores the mechanical energy storage of a carbon bundle made from a new class of ultra-thin carbon nanostructures - carbon nanothreads through a combination of large-scale molecular dynamics simulations and continuum elasticity theory. Our previous studies show that carbon nanothreads have a structural-dependent ductility [4], and a tailorable thermal conductivity [5]. They also exhibit an order of magnitude higher interfacial shear strength than carbon nanotube (CNT) bundles due to the irregular surface-induced stick-slip motion [6]. Based on the analyses of two representative nanothread bundles, it is shown that their gravimetric energy density decreases with the number of filaments, and torsion and tension are the two main deformation modes. Torsion dominates the energy storage at small torsional strain, especially for the bundles with small number of filaments. For larger bundles, tensile deformation is the predominant determines energy storage mode. Our results show that nanothread bundles have similar mechanical energy storage capacity to CNT bundles but exhibit their own advantages. The intrinsic structure of nanothread allows us to realize the full mechanical energy storage potential of its bundle structure through a pure tension, with a gravimetric energy density of up to 1.76 MJ/kg. This is 4 to 5 orders higher than steel springs and up to 3 times compared to Li-ion batteries. With their high energy storage density, fully hydrogenated surface features, large structural variety and highly tailorable mechanical properties, our work suggests that nanothread bundles are promising alternative building blocks for energy storage devices.

Keywords: Carbon Nanothread; Carbon Nanofiber; Mechanical Energy Storage; Mechanical Deformation; Molecular Dynamics Simulation

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