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Nano-architected metamaterials: Carbon nanotube-based nanotrusses

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ABSTRACT

In this paper, we propose a novel face-centered cubic (fcc) lattice-like nanotruss with carbon nanotubes and newly designed 12-terminal junctions as building blocks. Using molecular dynamics simulation, both thermal and mechanical properties of this novel nano-architected metamaterials are systematically predicted and a comparison study is conducted between fcc and simple cubic lattice-like nanotrusses. Our findings demonstrate that the fcc lattice-like nanotrusses have relatively low thermal conductivity $\kappa = 1.24 \sim 3.31 W/(m{\cdot}K)$ and reasonably high specific modulus $M = 49.79 \sim 114.15 MN{\cdot}m/kg$ in all three directions ([100], [110], [111]), for a material density in the range of $\rho = 0.23 \sim 0.82 g/cm^3$. Depending on the specific requirements in material design, the widely ranged Young's modulus E and thermal conductivity κ of nano-architected metamaterials can be tuned by changing the tube length. All the aforementioned advantages can be maintained at a high temperature up to $3000K$, which indicates fcc lattice-like nanotrusses are superior to most existing mechanically robust thermal insulators. To showcase the scale independency of the unprecedented properties of the proposed nano-architected metamaterials, thermal and mechanical properties of their macroscopic counterparts are studied using standard mechanics multiscale homogenization.

1. Introduction

Low-dimensional nanomaterials, like one-dimensional (1*D*) carbon nanotubes (CNTs) [1] and two-dimensional (2*D*) graphenes [2], have attracted considerable attention from material scientists and engineers, owning to their outstanding features, such as extremely high thermal conductivity [3–6], excellent mechanical strength [7–9], chirality-dependent electrical conductivity [10–12], and large specific surface area [13]. These unprecedented properties, however, are only observed along specific directions, *e.g.* tube axial direction for CNTs and plane direction for graphenes.

3*D* carbon nanotube networks [14], which employ various junctions [15] to link CNTs covalently, are emerging as one of the most promising lightweight multifunctional materials and have recently attracted considerable research interest, since they are aligned with the growing research efforts on architected cellular solids [16] and cellular-based metamaterials [17]. Earlier studies have reported various types of junctions, including the 3-terminal *Y*- and *T*-junctions [18–20], 4-terminal *X*-junction [21,22], and a few 3*D* multi-terminal junctions [23,24]. Some studies have also implemented fullerene-based junctions to assemble carbon nanotubes [25]. These junctions have been successfully synthesized in experiments utilizing various approaches: electron or ion beam welding [20,26,27], chemical vapor deposition [28], arc discharge [29] and nanochannel alumina [30]. Assembling single-walled carbon nanotubes (SWCNTs) by the junctions, different types of carbon nanotube networks can be developed, such as super carbon nanotubes [31], stacked hexagonal superarchitectures [32], super-cubic nanotrusses, and superdiamond nanotrusses [32–34]. These CNT networks not only extend some excellent properties of low-

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dimensional nanomaterials to three dimensions but also possess many extraordinary properties which their constitutive building blocks do not possess. For instance, 3D CNT networks are one of the best candidates for hydrogen storage due to their low density, large surface area, and continuous porosity [35–37]. The unique thermal properties and electrical rectifying effect make these nanotube networks a promising material for next-generation thermal management [38,39] and electronic [40–42] nanodevices, respectively. In addition, 3*D* CNT networks can be applied as strain sensors due to their durability and high sensitivity to strain [43].

Inspired by the ceramic nanolattice structures introduced by Meza et al. [44], we propose a novel face-centered cubic (fcc) lattice-like hollow nanotruss which consists of 12-terminal junctions and (8,8) armchair SWCNTs. In order to synthesize a *Y*-junction, Terrones et al. [45] removed one of the "arms" of an *X*-junction by using careful conditions of irradiation, which indicates that three, four, or even more terminals can be generated with controlled electron irradiation. Despite the fact that several studies have investigated both thermal and mechanical properties of simple cubic (sc) and body-centered cubic (bcc) lattice-like nanotrusses [23,25,33,34], there is a lack of knowledge about thermal and mechanical properties of the CNT-based fcc lattice-like nanotruss. To the best of our knowledge, the only recent paper studied the fcc lattice-like structure [46] is based on graphenes rather than nanotubes, which built the nanotrusses in a different way from our proposed model; the paper merely discussed mechanical properties and focused on compression tests. The unit-cell length in the aforementioned study was fixed at 5.5 *nm*, in which the properties of the nanotruss are still dominated by the junctions rather than the architecture. In this work, we construct fcc lattice-like nanotruss based on (8,8) single-walled carbon nanotubes. Using molecular dynamics (MD) simulation, both thermal and mechanical properties (including thermal conductivity, Young's modulus, specific modulus, initial fracture strain, initial fracture strength, and ultimate strength) of fcc and sc lattice-like nanotrusses are obtained. For convenience, these two nanotrusses are termed as SC and FCC hereinafter, owing to their similarity to the simple cubic (sc) and face-centered cubic (fcc) crystal structures, respectively. We focus on the architecture rather than the junction configuration, and the length of SWCNTs is changed over a wide range. Tensile tests are conducted in [100], [110] and [111] directions. Thermal and mechanical properties of the FCC nanotruss are compared with the SC nanotruss. The observation demonstrates that FCC nanotrusses can be employed as lightweight and mechanically robust thermal insulators with tunable Young's modulus, thermal conductivity and high thermal stability.

2. Model and computational method

2.1. Model

Unit cells of the SC and FCC nanotrusses are illustrated in Fig. 1a and f, respectively. We covalently join the (8,8) SWCNTs together by introducing topological defects, *e.g.* pentagonal and heptagonal rings, into perfect hexagonal nanotubes to generate junctions. In terms of the SC nanotruss, each junction connects 6 SWCNTs covalently, and consequently, a 6-terminal junction is named (Fig. 1b and c). There are 8 three-tube-constructed surfaces in each junction with three heptagons in every surface, and thus 24 heptagons are presented in total (colored in green). This SC nanotruss has the same architecture of the one considered in Refs. [23] and [47]. Furthermore, the FCC nanotruss consists of 12 terminals per junction, *i.e.* a 12-terminal junction (Fig. 1g and h). The defects in this type of junction can be categorized into two parts: (1) eight three-tube-constructed surfaces with three heptagons per surface, similar to the 6-terminal junction (colored in green) and (2) six four-tube-constructed surfaces with six heptagons per surface (colored in red), so the 12-terminal junction contains 60 heptagons in total.

It should be noted that these junctions can have a variety of configurations, as long as the number of non-hexagonal rings obeys Euler's law for polygon [49] and each carbon atom has three covalent bonds (see the Supporting Information S1 for details). Different junction configurations can give rise to changes in mechanical behaviors [21]. In this work, however, we only employ the junctions described in Fig. 1, and all the nanotubes are (8,8) armchair carbon nanotubes. We focus on the dependence of thermal and mechanical properties on the architecture rather than the junctions, because compared with the junction configurations, the architecture has a greater influence on the overall properties of these nano-architected metamaterials [33]. Although, more technological advancements are needed to synthesize 3D CNT networks as ideal as Fig. 1, our study can still explore the properties of nano-architected materials and shed lights on the fabrication and application of these novel nanomaterials. Advances in 3D printing technology, *e.g.* direct-laser-writing optical lithography [50], have also made it possible to fabricate nanoscale materials with complex architectures.

MD simulation is performed on six sets of SC and FCC nanotrusses with different SWCNTs lengths. For further discussion, we distinguish our systems in terms of "SC-*N*" and "FCC-*N*" terminology, where *N* represents the number of the hexagon rings in each nanotube connecting adjacent junctions, as can be seen in Fig. 1d,i. Six different tube-length-parameters ($N = 3, 7, 12, 16, 20, 24$) are chosen in this study corresponding to a wide range of tube length. The atom number and density of SC-*N* and FCC-*N* unit cells are listed in Supporting Information S2. As the tube length parameter *N* increases from 3 to 24, the density of the FCC nanotrusses decreases from $0.82 g/cm^3$ to $0.23 g/cm^3$, which is much smaller than that of SWCNTs ($\rho_{SWCNTs} \approx 2.27 g/cm^3$).

2.2. Computational method

Thermal and mechanical properties of the SC and FCC nanotrusses are simulated using LAMMPS package [51] with AIREBO potential [52]. Applying a reverse non-equilibrium molecular (rNEMD) algorithm of Muller-Plathe [53], thermal conductivities are calculated, and mechanical properties are simulated by utilizing the quasi-static displacement-controlled deformation method. Thermal properties are simulated along the [100] direction; mechanical properties are simulated along the [100], [110], and [111] directions. These three directions are represented by solid black arrows in Fig. 1e. Owing to the symmetry of the unit cells, the [100], [010], and [001] directions are equivalent; the [110], [101], and [011] directions are equivalent. Details of thermal and mechanical simulation are documented in Supporting Information S3. To verify our simulation procedure, the properties of a single $(8, 8)$ SWCNT are simulated using the same aforementioned methods and compared with previous studies (Supporting Information S4). It should, however, be noted that bond-breaking behavior is hard to be precisely captured with empirical potential functions used in MD simulation [54] and it is generally accepted that fracture strain and fracture strength calculated from MD simulation are less accurate than for Young's modulus obtained near the equilibrium state [25,54]. Nevertheless, the fracture patterns of CNT are still in accordance with the experimental findings [25], and therefore all the fracture behavior observed in this paper are qualitatively analyzed.