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Mechanical analysis of graphene-based woven nano-fabric

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ABSTRACT

Tailoring and assembling graphene into functional structures with well-defined configurations has been emerging as a key way for utilizing it in many promising applications. Here we report a graphene-based woven nano-fabric (GWNF) composed of graphene nanoribbons (GNR) which are interlaced with each other in an over and under fashion. Simulation results inform that the mechanical properties of GWNF can be tuned by the weave density of GNRs. Compared with pristine graphene, GWNF demonstrates a significantly enhanced flexibility with outstanding toughness and unprecedented energy-absorption capability. Shear forces from adjacent GNRs exert a negative impact to deteriorate the stretch capability of GWNF. Through the pull-out test of single central GNR, GWNF with inherent curvatures and defects leads to a riveting inter-locking phenomenon followed by a pronounced jump of pull-out force. GWNF with a high density of GNRs reproduces mechanical properties similar to graphene via nanoindentation while GWNF with a low density of GNRs exhibits an extraordinary toughness unmatched by graphene. These intriguing mechanical properties of GWNF insinuate that it can serve as a solid building block to envisage a large variety of applications such as composites, strain sensors, and solar cells by taking advantages of the special woven structure.

1. Introduction

The creation of self-assembled complex structures and their peculiar functions are both of great scientific interest and importance. In the past decade, carbon nanotubes have been successfully incorporated into various macroscopic structures such as yarns [1], ribbons [2], and sheets [3,4] with many unique applications based on their extraordinary properties. For instance, cross-stacked superaligned carbon nanotube films with anisotropic mechanical properties were reported to make transparent and stretchable conductors [5]. Macroscopic uniform graphene ribbons with high flexibility have been controllably fabricated by a modified wet-spinning method [6]. The hydrogenation of pristine graphene sheets can create three dimensional complex structures, such as nanohelices [7], nanocages [8], and folded graphene origami [9]. Recently, to imitate the structure of textiles, a woven nanostructure made of individual CNTs has been proposed and envisioned as a promising candidate for aerospace products due to its superb toughness, strength, and lightness [10]. The synthesis of porous carbon or multi-layer graphene/porous carbon woven composite films into fabrics creates new platforms for fiber supercapacitors [11,12]. The nanotube fibers are woven into textiles to make promising electronic-textile applications including distributed sensors and electronic interconnects, among others [13]. Surface-initiated assembly has been employed to engineer multiscale, free-standing nanofabrics using a variety of extracellular matrix proteins (fibronectin, laminin, fibrinogen, collagen type I and collagen type IV) [14]. A graphene-based woven fabric (GWF) has been prepared on a woven copper mesh template by interlacing two sets of graphene micro-ribbons with the ribbons intersecting each other at essentially right angles by utilizing chemical vapor deposition. The GWF displays good dimensional stability in both the warp and weft directions and the observed combination of film transparency and conductivity can be optimized by tuning the ribbon packing density [15]. GWF undergoes significant changes in its polycrystalline structure and exhibits high density of crack formation and propagation when mechanically deformed. The electrical resistance of GWF increases exponentially with tensile strain by a gauge factor of $\sim 10^3$ under 2–6% strains and $\sim 10^6$ under higher strains. These strains are the highest thus far reported due to its unique fabric-like woven mesh configuration and sensitive fracture behavior, which make it an ideal structure for sensing tensile deformation by changes in strain [16]. However, molecular dynamic studies have never been performed to study woven fabric-like nanostructures composed of graphene nanoribbons. Here we report molecular dynamics simulation results for GWNF which is assembled by orthogonally intersecting GNRs. The woven density of GNRs is the key to create the different models.

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Through the stretch, pull-out and nanoindentation test, we intend to investigate the mechanical properties of GWNF from a variety of viewpoints and make comparisons with graphene. It is envisioned that the periodic voids in the GWNF can be filled with other functional materials, or serve as a semipermeable membrane or filter for reverse osmosis or cell applications. Also GWNF can create a platform to bolster a large variety of applications such as composites, strain sensors, and solar cells by taking advantages of the special structure of woven materials and the properties of graphene.

2. Computational model and methodology

In the simulation, in order to model bond formation and breaking in the system we have used the adaptive intermolecular reactive empirical bond order (AIREBO) potential [17]. It should be noted that this potential is best suited for systems containing hydrogen and carbon, which makes it accessible for all-carbon systems such as the ones being modeled here. The AIREBO potential can be expressed as

$$E=\frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{REBO}+E_{ij}^{LJ}+\sum_{k\neq i,j}\sum_{l\neq i,j,k}E_{kijl}^{TORSION}\right] \quad (1)$$

where the E^{REBO} term is the REBO potential [18], shown as

$$E_{ij}^{REBO}=V_{ij}^{R}(r_{ij})+b_{ij}V_{ij}^{A}(r_{ij}) \quad (2)$$

where V^R is a repulsive term, V^A is an attractive term, and b_{ij} is the environmental-dependent bond order term between atoms which activates the attractive term only for bonded atoms. Since the REBO potential only accounts for the interactions of atoms within two Angstroms of one another, the AIREBO potential also includes the E_{LJ} term, which is a standard 12-6 Lennard Jones potential for distances 2 Å $< r <$ cutoff, given here as

$$E_{LJ}=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right] \quad (3)$$

where ϵ is the depth of potential well, σ is the finite distance where the potential is zero, and r is the distance between the particles. The cutoff for the LJ term is set here to be 2.5σ as a good balance between computation speed and accuracy. The AIREBO potential also includes the $E^{TORSION}$ term, which is a four-body potential enforcing hydrocarbon dihedral angle preference. The conjugate gradient algorithm has been employed to perform the energy minimization until the total energy change between two successive iterations divided by the energy magnitude is less than or equal to 10^{-8}. After the equilibrium state is achieved, NVT ensemble (the number of particles in the system, system's volume,

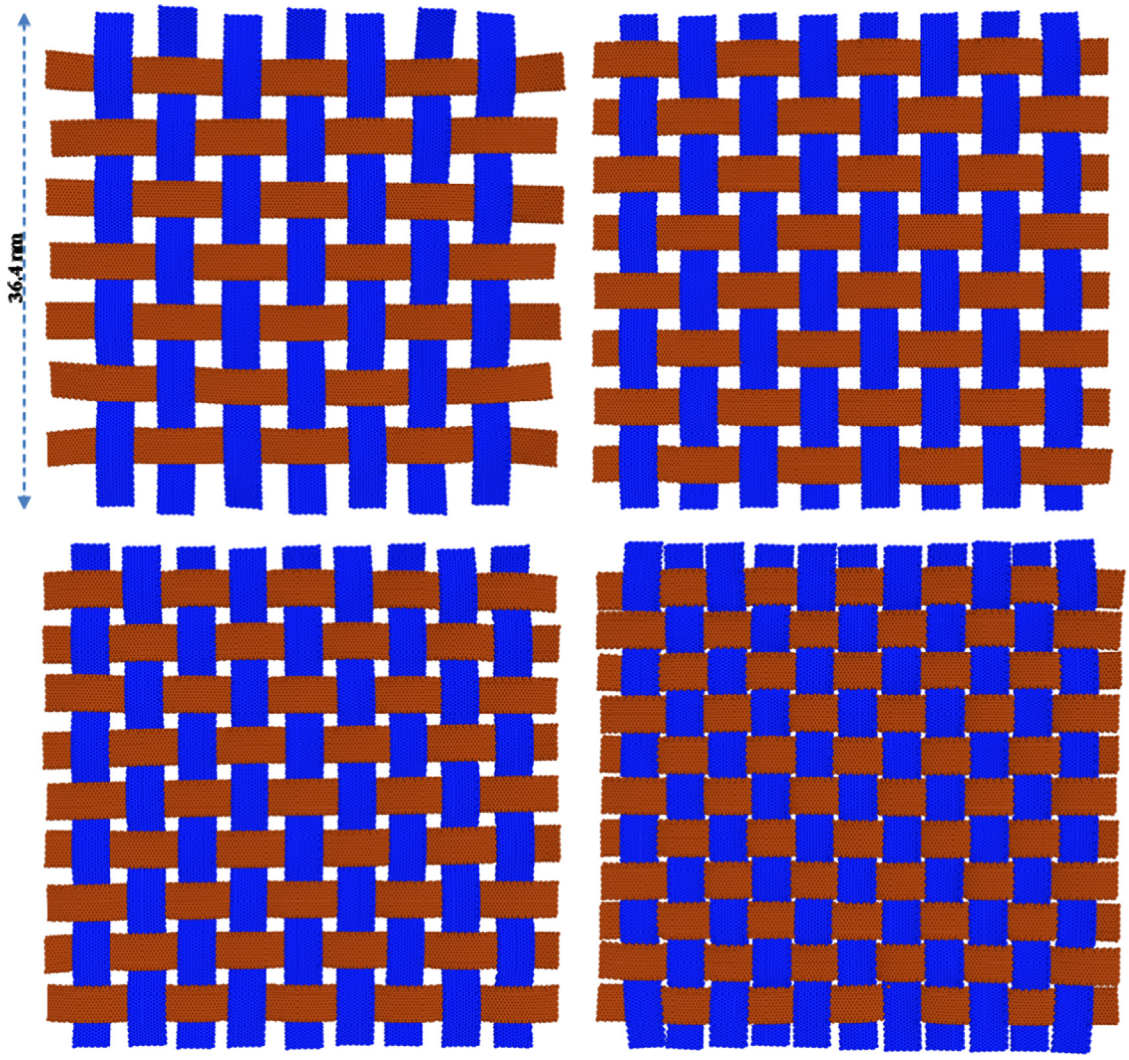

Fig. 1. GWNF molecular dynamics simulation models with 7×7, 8×8, 9×9 and 11×11 GNRs. The brown color shows the GNRs orient along the horizontal direction (x-axis), the blue color shows the GNRs orient along the vertical direction (z-axis). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)