Mechanical analysis of graphene-based woven nano-fabric

Liuyang Zhang, Matthew Becton, Xianqiao Wang *

College of Engineering and NanoSEC, University of Georgia, Athens, GA 30602, USA

A R T I C L E   I N F O

Article history:
Received 16 July 2014
Received in revised form 10 October 2014
Accepted 14 October 2014
Available online 22 October 2014

Keywords:
Graphene woven nano-fabric (GWNF)
Graphene nanoribbons (GNR)
Molecular dynamics simulation
Toughness
Pull-out

A B S T R A C T

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 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.

© 2014 Elsevier B.V. All rights reserved.

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 $\sim 10^5$ 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 GWF which is assembled by orthogonally intersecting GNRs. The woven density of GNRs is the key to create the different models.
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

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

where the \( E_{\text{REBO}}^{ij} \) term is the REBO potential \[18\], shown as

$$ E_{\text{REBO}}^{ij} = V_R^{ij}(r_{ij}) + b_i V_A^{ij}(r_{ij}) $$

where \( V_R^{ij} \) is a repulsive term, \( V_A^{ij} \) is an attractive term, and \( b_i \) 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 \( E_{\text{LJ}} \) term, which is a standard 12-6 Lennard Jones potential for distances \( 2 \sigma < r < \sigma \), given here as

$$ E_{\text{LJ}} = 4 \epsilon \left[ \frac{\sigma_{12}}{r} - \frac{\sigma_{6}}{r^6} \right] $$

where \( \epsilon \) is the depth of potential well, \( \sigma \) 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 \( 2.5 \sigma \) as a good balance between computation speed and accuracy. The AIREBO potential also includes the \( E_{\text{TORSION}} \) 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,
absolute temperature) simulations with a constant temperature of 1 K are carried out based on the Berendsen thermostat and Newtonian equations of motion. All the simulations are performed with the LAMMPS package [19].

In this paper, the GWNF is composed of interlaced $7 \times 7$, $8 \times 8$, $9 \times 9$, or $11 \times 11$ GNRs with chirality (6,6) as depicted in Fig. 1. Energy minimization simulation shows that the GWNF is stable under temperature 1 K. The in-plane motion of single GNR in GWNF is partially constrained by the woven structure. We also have not observed any ripple phenomenon in the woven model due to the enhanced bending rigidity of the GWNF system comparing with a single-layer graphene system. The square surface area for each GWNF is identical with an edge length of 364 Å. The side length of the square periodic holes in the lattice are, in order of increasing density of GNRs, about 22.11 Å, 18.9 Å, 15.8 Å and 8.0 Å respectively. GWNF can be regarded as a thin film teemed with uniformly distributed square-shaped defects. The distance between the two GNRs at the joint position is about 3.4 Å which is the equilibrium interlayer distance of graphite. The interaction between the GNRs is described by Eq. (3) using $\sigma = 3.36$ Å and $\epsilon = 2.168$ meV as demonstrated for the interaction between two graphene sheets with a turbostratic orientational relationship [20]. We perform a series of mechanical tests, such as the impact test with a CNT at a 45° tilt angle, a single GNR pull-out test, a bidirectional stretch test, and an indentation test, in order to investigate the mechanical properties of the GWNF. Constant velocity in steered molecular dynamics (SMD) [21] is applied through a virtual spring attached to dummy atoms for the stretch and pull-out tests. The force $F$ needed for the displacement of the dummy atoms to an imaginary point can be calculated by the following equations:

$$F = -\nabla U$$

(4)

Fig. 2. Impact test of (a) $7 \times 7$, (b) $9 \times 9$, (c) $11 \times 11$ GWNFs, (d) single-layer graphene, and (e) two-layer graphene. Column (I) represents the atomic potential map of initial state. The carbon nanotube is placed at the same height for each test. Column (II) represents the atomic potential map of final snapshot. Column (III) represents the zoom-in profile at the penetration position. The color bar depicts the range of the potential energy of each atom.
where \( VU \) is the potential energy gradient, \( k \) is the spring force constant, \( v \) is the velocity of pulling, \( t \) is the current time, \( r \) is the instantaneous vector position, \( r_0 \) is the initial vector position of the SMD atom and \( n \) is the vector direction in which the dummy atom is displaced.

\[
U = \frac{1}{2} k [v(t) - (r - r_0) \cdot n]^2
\]

(5)

3. Results and discussions

3.1. Impact test

From the energetic perspective, penetrating the GWNF requires sufficient effort to overcome the fracture energy barrier. The impact of high velocity carbon nanotube (CNT) provides a feasible way for transferring sufficient kinetic energy to the GWNF to surpass this barrier. Interesting questions of what initial velocity is required to pierce through the GWNF and how it compares to pristine graphene remain to be further explored. In what follows, we devise a simulation test in which a CNT tilted 45° to the direction of the weave is directed toward the GWNF from a distance 100 Å away along the \( y \)-axis with an initial velocity varying from 100 Å/ps to 550 Å/ps. Three individual runs are performed for each specified initial velocity of CNT so as to average the simulation results and lessen the uncertainty from the computational errors.

Fig. 2 shows comparisons of the critical initial velocities for penetrating the different density weaves of GWNF and also a graphene sheet with the same size. To begin, the initial penetration velocity for a single layer of graphene is estimated to be 185 Å/ps from MD simulation. With the same initial velocity for the \( 7 \times 7 \) GWNF, the CNT is unable to penetrate and bounces back, indicating that the GWNF possesses a larger capacity to absorb the impact energy than the pristine graphene sheet. The flexibility of the interwoven warp and weft graphene nanoribbons in the GWNF allows the energy to spread out inside the structure. For the \( 7 \times 7 \), \( 9 \times 9 \), and \( 11 \times 11 \) GWNFs, the critical penetration velocities increase from 300 Å/ps, 360 Å/ps to 400 Å/ps as the weave density does. The high density of \( 11 \times 11 \) GWNF spreads out the impact energy (99.58 kev) more efficiently than \( 7 \times 7 \) (56.01 kev) and \( 9 \times 9 \) (80.66 kev) GWNF. In terms of thickness and effective area, the \( 11 \times 11 \) GWNF is close to the structure of two-layer graphene, however the critical velocity required is 700 Å/ps to penetrate the two-layer graphene. This is explainable because two layers of graphene have a larger overlapped contact area between the layers which allows for a maximum transfer of impact energy (304.96 kev). On the other hand, the initial velocity needed to rupture the \( 11 \times 11 \) GWNF is 2.2 times greater than single layer graphene which offers an avenue for producing an efficient energy absorber based on GWNF structures.

3.2. Pull-out test

To check the binding interaction between the GNRs inside the GWNF structure which plays a key role in holding the integrity of the structure under a variety of circumstances, we intend to pull out the central GNR from the GWNF by using SMD. Three types of GWNF: \( 7 \times 7 \), \( 9 \times 9 \), and \( 11 \times 11 \) are studied as shown in Fig. 3. A small rectangular area (364 Å × 47 Å) of three sides of the GWNF is fixed, while the rest side of the GWNF remains free to move. The extraction velocity is set to be 1 Å/ps. At the beginning, a large force of 5 nN is needed to initialize the pull-out process which is similar to the uncramping stage for the extraction of a single yarn from fabric at macroscopic level [22]. When the entire GNR begins to translate within the GWNF swath, the pull-out force gradually decreases. According to the atomistic simulations of sliding friction of graphene flakes, the average dynamical friction force during the pull-out motion is smaller than the static friction force [23] just as with macroscopic phenomena in which the dynamic and static friction coefficients play a significant role in determining behavior. The curves in Fig. 3 show that the pull-out force of a single GNR from the GWNF varies slightly between different densities of GWNF due to the small friction between the GNRs for three types of GWNF after the GNR moves. The low woven density of \( 7 \times 7 \) GWNF makes it easy to pull out because of a small number of cross-yarns. For the high density \( 9 \times 9 \) and \( 11 \times 11 \) GWNF, an

![Fig. 3. Pull-out forces of \( 7 \times 7 \), \( 9 \times 9 \), and \( 11 \times 11 \) GWNFs evolves with simulation time. (a) Inter-locking phenomenon between GNRs in \( 9 \times 9 \) GWNF, in which atoms enclosed in the red region are fixed during the simulation.](image-url)
interesting phenomenon of interlocking at cross-yarns of GNR is observed as shown in Fig. 3. The edges of the extracted GNR are locked by the edges of the vertical GNRs which in turn lead to a large peak pull-out force in the curves. With more cross-yarns encountered during the pull-out process, a higher possibility of interlocking at a crossing point happens. The interesting pull-out simulation indicates the inherent curvature of GNRs and square-shaped defect behavior of GWNF which affect the intramolecular friction between the GNRs and load effects on the pull-out force.

3.3. Stretch test

The strength of woven structures is enforced by the presence of the crossing points, where warp and weft yarns interlace with each other to form a fabric. In contrast to flat graphene, GWNFs can undergo significant changes when mechanically deformed. When a fabric is under uniaxial or biaxial tension or 45° direction tension, the yarn-yarn interactions at the crossing points are eligible to undergo readjustment, shifting the relative position of the GNRs. Here we discuss the critical behavior when a tensile load is applied along the biaxial direction by using SMD for $7 \times 7$, $8 \times 8$ and $9 \times 9$ GWNFs and also for single layer graphene. The virtual spring exerts force on the GNRs which in turn deform during the stretching process. Fig. 4 shows the force and displacement relationship of GWNFs and graphene during a biaxial stretch test. The slope of these curves at the early stage shows that graphene is stiffer than the GWNFs, but less tough overall. For graphene, the force reaches 448 nN before fracture occurs as shown in Fig. 4(a). As the number of woven GNRs increase from 7 to 9, the GWNF displays intriguing mechanical properties. $7 \times 7$ GWNF has the largest deformation and sustains the loading until 1205 nN before fracture compared to $8 \times 8$ GWNF (1022 nN) and $9 \times 9$ GWNF (670.4 nN). The GWNF breaks spontaneously when the fracture happens as shown in Fig. 4(b). The number of cross-yarns has a

![Fig. 4. Force–displacement relationship of $7 \times 7$, $8 \times 8$, $9 \times 9$ GWNFs, and single layer graphene under biaxial stretch. (a) Critical snapshot when fracture in graphene appears. (b) Failure pattern when fracture in $7 \times 7$ GWNF occurs. The fracture behavior for $8 \times 8$ and $9 \times 9$ GWNFs are similar to $7 \times 7$ GWNF.](image)

![Fig. 5. Schematic views of single GNRs in the (a) $7 \times 7$, (b) $8 \times 8$ and (c) $9 \times 9$ GWNFs. The blue arrows represent the normal direction of forces from GNRs orthogonal to the current one. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)](image)
pronounced effect on the strength and toughness of the GWNF. The strength of GWNF is deteriorated by the alternate shear effect between adjacent GNRs in the orthogonal direction as shown in Fig. 5. It can be explained by two factors. As the number of cross-yarns increases, for instance 7 × 7 GWNF to 9 × 9 GWNF, the shear force exerted on the curvature at short distance makes the GWNF facile to break during the stretch test. Besides, as the deformation of GWNF increases, the repulsive force following the shortening distance between two orthogonal GNRs causes the increment of shear forces and high possibility of breakage.

Toughness is the ability of a material to absorb energy and plastically deform without fracturing which balances the strength and ductility of material. Strictly, toughness is defined as the amount of energy per volume,

$$T_{\text{material}} = \frac{\text{Energy}}{\text{Volume}} = \int_0^{\varepsilon_f} \sigma d\varepsilon = \frac{\int_0^{\varepsilon_f} F \, du}{\text{Volume}}$$  \hspace{1cm} (6)

where $\varepsilon$ is the strain, $\varepsilon_f$ is the strain upon failure, $\sigma$ is the stress, $F$ is the force, $u$ is the displacement, and $u_f$ is the displacement upon failure. Table 1 shows the toughness of graphene and GWNFs. The toughness of GWNFs is 1.8–4.8 times greater than graphene which indicates its potential use for absorbing or transferring mechanical energy.

The woven GNRs are non-covalently bonded at the cross point which endows the inherent tunable morphology. To demonstrate its unique flexible configuration, the 7 × 7, 9 × 9, and 11 × 11 GWNFs are stretched in the 45° direction by using SMD attaching two diagonal angles. The boundary of GWNF is capable to move freely. The relationship of force displacement is depicted in Fig. 6.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Toughness (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphene</td>
<td>2.93</td>
</tr>
<tr>
<td>9 × 9 GWNF</td>
<td>5.27</td>
</tr>
<tr>
<td>8 × 8 GWNF</td>
<td>12.48</td>
</tr>
<tr>
<td>7 × 7 GWNF</td>
<td>14.17</td>
</tr>
</tbody>
</table>

The initial force to tilt the GWNF is 13 nN for 11 × 11 GWNF, 12 nN for 9 × 9 GWNF, and 8.8 nN for 7 × 7 GWNF which indicates that the high density of local deformation of GNRs causes the GWNF difficulty in changing its structure. Fig. 6(a–c) shows the final snapshots of 7 × 7, 9 × 9, and 11 × 11 GWNFs. The simulations stop at a displacement of 100 Å where the woven GNRs are pulled out from the GWNF. The 7 × 7 GWNF has a loose cross-yarn which displays a very irregular shape after the deformation. The inter-GNRs’ binding in 7 × 7 GWNF is weak compared with 9 × 9 and 11 × 11 GWNF, which makes the transfer of external load insensitive before the GNRs are pulled out from the sides of GWNF. For 9 × 9 and 11 × 11 GWNFs, the translocations and shape change of the holes from rectangles to parallelograms are easily observed due to strong inter-sheet binding. The sliding of the cross-yarns changes the rectangular GWNF to a parallelogram structure. Intuitively, the 11 × 11 GWNF that has the densest cross-yarns needs a larger force to deform its structure. However, during the deformation the stretch force for 7 × 7, 9 × 9, and 11 × 11 GWNFs fluctuates at the same amplitude as single GNR pull-out test which further indicates the weak vdW interactions between the GNRs. From the stretch test, the GWNF has astounding toughness which offers potential use for energy dissipater and stretchable electronic devices.

3.4. Nanoindentation

The two-dimensional graphene sheet can support a very large normal bending prior to the occurrence of fracture by using AFM to indent a graphene sheet suspended over a circular hole [24]. It is debatable whether a GWNF sheet is truly a two-dimensional structure since it exhibits out-of-plane yarns as compared to pristine graphene yet it has similar bending properties to graphene. Here for the purpose of comparison with graphene based on the mechanical properties such as 2-D elastic modulus, 2-D pre-tension we discuss as follows, the GWNF is treated as a two-dimensional structure. In order to carry out the nanoindentation MD simulation, a sphere with a radius of 59.2 Å constructed from graphite was introduced to serve as the indenter. The radius of the indenter is chosen to cover four holes of 7 × 7 GWNF, which has

Fig. 6. Force displacement relationship of 7 × 7, 9 × 9, and 11 × 11 GWNFs under 45° tilt stretch test. (a) Irregular shape of 7 × 7 GWNF after certain deformation. (b) and (c) Regular configuration of 9 × 9 and 11 × 11 GWNFs after certain deformation, respectively.
the lowest density of GNRs in our simulation. Nanoscale graphene woven structure is still challenging to fabricate comparing with the overlying graphene nanoribbon structure. Here we take the cases of 11 × 11 GWNF, 11 × 11 graphene over-under fabric (GOUF) and single layer graphene to show the differences between the GWNFs, GOUF, and graphene. The indenter is located above the center of the GWNF at a distance of 5.6 Å and is considered to be a rigid object so that the atomic configuration of the indenter does not change during the simulation. The indenter is moved at constant velocity of 0.2 Å/ps in the direction perpendicular to the GWNF surface as shown in Fig. 7(a). The atoms on the edge of the GWNF remain in a static equilibrium state due to the fixed boundary conditions. After enough loading time, the film is eventually heavily deformed by the indenter but it should be noted that the simulation does not run until the GWNF is pieced through by the indenter. The final state for the GWNF where the woven GNRs are distorted is shown in Fig. 7(b). Fig. 7(c) and (d) shows the final state for graphene and 11 × 11 GOUF which has same indenter depth as the GWNFs do.

Similar to the indentation experiments and simulation of circular and rectangular graphene [24,25], the formula to describe the relationship between indentation depth and load for GWNF is expressed as

$$F = F_s(d) + F_E(d)$$

where $d$ is the indentation depth and $F$ denotes the concentrated force experienced by the GWNFs. The load force consists of two parts: the first part, $F_s(d)$, represents the term due to the axial tension of the two dimensional GWNF,

$$F_s(d) = \sigma_0^{2D}(\alpha Requ)^{1/2} \left( \frac{r}{Requ} \right)^{3/4} \left( \frac{d}{Requ} \right)$$

where $\sigma_0^{2D}$ is the pre-tension of the single-layer GWNF, $r$ is the indenter radius, $\alpha$ denotes the aspect ratio and is equal to $\sqrt{1/b^2}$, in our case $\alpha = 1$, and $Requ$ represents the equivalent radius of the square GWNF, $\sqrt{1/b^2}$. The second term $F_E(d)$ represents the large deformation term,

$$F_E(d) = E^{2D}(q^2 Requ)^{1/2} \left( \frac{r}{Requ} \right)^{1/4} \left( \frac{d}{Requ} \right)$$

where $E^{2D}$ is the 2D elastic modulus of GWNF. The common pre-tension and elastic modulus of a 3-D bulk material can be obtained through the 2-D pre-tension and elastic modulus divided respectively by the effective thickness which is always treated as the layer spacing of graphite crystal, 3.4 Å. In addition, $q$ is a dimensionless value, $q = 1/(0.15 - 0.15\alpha - 0.16\alpha^2) = 0.9795$, where $\alpha$ denotes Poisson’s ratio, for graphene $\alpha = 0.165$ [24]. It is reported that when $r/R > 0.1$, the indenter radius has a significant influence on the load–displacement properties. In our simulation, $r/R > 0.1$, thus, Eqs. (8) and (9) are corrected by a factor of $(r/R)^{3/4}$ and $(r/R)^{1/4}$ respectively [25].

The load–displacement curves in Fig. 7 can be attained from the cross-dependence of indenter load and indentation depth. According to Eq. (7), the nonlinear least-square method is used to fit the simulation results. The pre-tension and elastic modulus calculated from the results are shown in Table 2, which are in agreement

![Fig. 7. Load histories of 11 × 11 GWNF and single layer graphene vs. the indentation depth. (a) Indentation model for 11 × 11 GWNF, (b-d) Final snapshot for 11 × 11 GWNF, graphene and 11 × 11 GOUF during the indentation process.](image)

**Table 2**

Mechanical properties of graphene and 11 × 11 GWNF from nanoindentation simulations.

<table>
<thead>
<tr>
<th></th>
<th>2-D elastic modulus (N/m) [25]</th>
<th>3-D elastic modulus (TPa) [25]</th>
<th>2-D elastic modulus (N/m)</th>
<th>3-D elastic modulus (TPa)</th>
<th>2-D pre-tension (N/m)</th>
<th>3-D pre-tension (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphene</td>
<td>353.0589</td>
<td>1.0539</td>
<td>430.28</td>
<td>1.27</td>
<td>18.94</td>
<td>55.71</td>
</tr>
<tr>
<td>11 × 11 GWNF</td>
<td>–</td>
<td>–</td>
<td>428.65</td>
<td>1.26</td>
<td>6.83</td>
<td>20.09</td>
</tr>
<tr>
<td>11 × 11 GOUF</td>
<td>–</td>
<td>–</td>
<td>379.91</td>
<td>1.12</td>
<td>13.68</td>
<td>40.24</td>
</tr>
</tbody>
</table>
with experimental results (1 ± 0.1 TPa) of the nanoindentation of freestanding monolayer circular graphene membranes [24] and the numerical result (1.04 TPa) of the nanoindentation of single layer rectangular graphene film [25]. The 2-D pre-tension depends on the loading speed of indenter and the indenter size. The 11 × 11 GOUF can sustain larger loading compared with 11 × 11 GWNF because the strength of GWNF is deteriorated by the alternate shear effect between adjacent GNRs in the orthogonal direction as explained in Fig. 5. The 3-D elastic modulus of 11 × 11 GWNF and 11 × 11 GOUF with its relatively high density of woven GNRs, is close to the modulus of graphene. The simulations show that the GWNF possesses interesting mechanical properties and has the potential for various applications.

4. Concluding remarks

In this paper, we have performed molecular dynamics simulations to construct various types of GWNFs by weaving GNRs and also to investigate the mechanical properties of the constructed GWNFs in order to fully unravel the mechanisms behind the properties of the structure. Simulation results have demonstrated that the weave density plays a significant role in the mechanical behavior of the GWNFs. GWNFs offer a promising way to enhance the toughness of graphene-based structures while maintaining the comparable strength of structures. An interesting inter-locking phenomenon is observed when a single central GNR is pulled out from GWNF indicating the inherent curvature and defect propensity of GWNF. GWNF with a high density of GNRs exhibits mechanical properties similar to graphene. Our proposed weaving structure is the most common plain woven pattern which has been utilized in a variety of applications. We also have other potential weaving patterns such as twill pattern, satin pattern, basket pattern, leno pattern, mock leno pattern etc. Take satin pattern for example, its weaves are fundamentally twill weaves modified to produce fewer intersections of warp and weft however it is unstable and asymmetric which could cause one face of the fabric to have fibers running predominantly in warp direction while the other face has fibers running predominantly in the weft direction. From the modeling viewpoint, more attentions should be paid to assemble multiple GNRs into different patterns such that residual stresses are not built into the components through an innovative assembly. These findings in this paper provide computational guidelines to study both GWNFs and the mechanical properties of GWNF-based composite materials and applications.

Competing financial interests

The authors declare no competing financial interests.

Acknowledgments

The authors acknowledge the support from the University of Georgia (UGA) Startup Fund. The facility support for modeling and simulations from the UGA Advanced Computing Resource Center are greatly appreciated.

References