In-plane compressive behavior of graphene-coated aluminum nano-honeycombs

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1. Introduction

As a type of novel lightweight materials, nano-honeycomb materials have attracted much attention in different fields such as chemistry [1], physics [2] and engineering [3] due to the combination of structural optimization of honeycomb materials and the excellent properties of nanomaterials [4,5]. Nano-honeycomb materials can be used for nanowire fabrication and as structural supports for devices [6,7]. Masuda and Fukuda [8], and Chu et al. [9] have successfully produced highly ordered alumina nanofilms with cylindrical pores using the templating method.

The discovery of graphene [10] has stimulated enormous studies on carbon (C) nanomechanics because of their extraordinary strength, stiffness and low-density properties. Graphene holds promise for important applications as, for example, reinforcements in polymers [11], ceramics [12] and metal [13–15]. Wang et al. [13] fabricated aluminum composites reinforced with graphene nanosheets through a feasible methodology based on flake powder metallurgy, and found that the tensile strength of 249 MPa was achieved in the Al composites reinforced with only 0.3 wt% graphene nanosheets, which is 62% enhancement over the unreinforced Al matrix. By using mechanical milling and hot rolling, Shin et al. [14] found that with an addition of only 0.7 vol% few-layer graphene (FLG), the composite exhibits a tensile strength of ∼ 440 MPa, about twice higher than that of monolithic Al.

Al always severs in a complex environment. Coating is a popular way to protect Al products. Compared with alumina coatings, graphene coatings possess various unique properties that are more suitable for lightest and thinnest protective barriers of metal aviation components against stress corrosion as well as overheating and lightning stroke, due to their excellent electrical conductivity, heat resisting property, chemical inertness and transparency [16–19]. Chen et al. [16] and Prasai et al. [17] found that graphene coating can prevent the formation of any oxide on the protected metal surfaces (Cu, Ni, Cu/Gr, and Cu/Ni). This protection method offers significant advantages and can be used on many metals that catalyze graphene growth. Topsakal et al. [18] studied Al (1 1 1) surface with graphene coating by first-principles calculations and found that continuous coating of pristine graphene on reactive surfaces can provide an excellent protection from oxidation of reactive surfaces at nanoscale, and the weak protection caused by the defect of graphene can be solved by increasing the number of coating layers. Sharma et al. [19] studied graphene-Cu composites by using the MD simulation method and found that graphene can improve both Young’s modulus and thermal conductivity of the nanocomposites compared with pure Cu. Chemical vapor deposition (CVD) can produce high-quality graphene films on a metal (e.g., Cu, Ni, Pt or alloy) surface at high temperatures, and the films are then transferred to other substrates [20]. It should be noticed that the chemical reaction between Al and graphene leads to the formation of Al carbide (Al4C3) at a higher
temperature, which weakens the mechanical properties of graphene-Al composites [21]. However, the transferring method is difficult to fabricate for graphene-coated Al nanohoneycombs (ANHCs). Fortunately, the development of low-temperature graphene growth [22] has provided a possibility for graphene coating on inner walls of ANHCs.

Molecular dynamics (MD) simulations have been widely used to predict the mechanical properties of nanomaterials [23,24]. For traditional porous materials, classical expressions have been given by Gibson and Ashby [7] to predict the Young’s modulus and yield stress in terms of the relative density of the material, and the scaling constants can be fitted by finite element (FE) analysis [25]. It is important to notice that these constants are not suitable well in nanoporous materials due to the large surface-to-volume ratio [26,27]. Yuan and Wu [28] found that the Gibson-Ashby’s scaling law is still applicable in nanoscale, but the scaling constants should be determined from experimental or simulation results.

It is of great interest to explore the reinforcing effect of graphene in such nanostructured materials as nanohoneycombs. In this work, the in-plane compressive behaviors of GANHCs including single-layer graphene (SG) coated ANHCs (SGANHCs) and double-layer graphene (DG) coated ANHCs (DGANHCs) as well as pure ANHCs with different relative densities are firstly investigated via MD simulations. We also propose a modified Gibson-Ashby model to predict the in-plane Young’s modulus and compressive strength of GANHCs.

2. Methodology

When coated on the inner wall of cylindrical pores, a sheet of graphene can be curved into a one-dimensional structure, that is, a carbon nanotube (CNT). Hence, the graphene coating is substituted by a CNT in our model. Although the mechanical properties of CNT/Al composites were investigated by Silvestre et al. [29] and Choi et al. [30] via MD simulations, both studies focused on the prediction of the out-of-plane mechanical behavior. A representative volume element (RVE) (see Fig. 1) of ANHCs, SGANHCs and DGANHCs is chosen respectively for MD simulations to investigate the uniaxial compressive behavior of the RVE in the in-plane direction. Fig. 1 shows the perspective and top views of the RVEs for polycrystal ANHCs, SGANHCs and DGANHCs. The x and y axes are considered as the in-plane directions, and the z axis is the out-of-plane direction, as shown in Fig. 1. The sizes of all RVEs are 12 nm × 12 nm × 12 nm (Fig. 1a), with a through cylindrical pore in the center (as shown in Fig. 1b), coated with a single-walled carbon nanotube (SWCNT) (as shown in Fig. 1c and d) or a double-walled carbon nanotube (DWCNT) (as shown in Fig. 1e and f). The chirality of the CNTs in our simulations is armchair. The inner–outer combination of DWCNTs is accord with (n, n)@(n + 5, n + 5), which is the most stable structure among armchair CNTs [31]. The length of CNTs along the z axis is 12 nm. The compression direction is along the y axis which corresponded to three crystal orientations (monocrystral [1 0 0], [1 1 1] directions and polycrystalline). For the [1 0 0] compression direction, the x, y and z axes correspond to [0 1 0], [1 0 0], [0 0 1] directions, respectively. For [1 1 1] direction, the x, y and z axes correspond to [1 1 0], [1 1 1] and [1 1 2] directions respectively. As shown in Fig. 1, 12 grains are randomly distributed inside the bulk in the polycrystalline Al model. To investigate the influence of relative mass density, 7 classes of ANHCs with a center cylindrical pore of different radii are built. In each compressive direction, there are 7 groups, which have identical inner radius and coating type, as listed in Table 1. The relative density \( \rho_r \) of the RVEs is calculated by \( \rho_r = M_r / M_b \), where \( M_r \) is the relative atomic mass of the bulk and \( M_b \) is the relative atomic mass of the RVE. For simplicity, the mass of the graphene coating is not taken account into when \( \rho_r \) is calculated in GANHCs. All models are constructed by using Atomsk [32]. Atomic images are visualized via Ovito [33].

MD simulations are performed by means of the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [34]. The Al-Al interaction is commonly described by an embedded atom method (EAM) potential [35], and the binding interaction of C-C is described by the widely used adaptive intermolecular reactive empirical bond order (AIREBO) potential [36]. The Lennard-Jones (LJ) 12-6 potential is adopted to simulate interatomic forces between C and Al atoms and long range van der Waals (vdW) interaction between C atoms. The LJ interaction is written as \( U_{LJ}(r_i) = 4\varepsilon[(\sigma/r_i)^{12}-(\sigma/r_i)^6] \), where \( r_i \) is the distance between those atoms not forming bonds, \( \varepsilon \) is the well depth and \( \sigma \) is the size parameter, and \( r_c \) is the cutoff distance. The LJ interaction results.

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3. Results and discussion

3.1. Stress-strain curves

Fig. 2 shows the tensile and compressive stress-strain curves of the 1st group of samples (as listed in Table 1) for polycrystalline ANHCs, SGANHCs and DGANHCs, respectively. It can be seen from Fig. 2a that the in-plane tensile Young’s moduli, tensile strengths and tensile energy absorption of both SGANHCs and DGANHCs are much larger than those of the pure ANHCs without graphene coating. The in-plane compressive stress-strain curves of all samples including ANHCs, SGANHCs and DGANHCs are shown in Fig. 2b. All simulations are carried out at the temperature of 300 K. The step time in the MD simulations is taken as 1 fs.

The periodic boundary conditions are applied in all three directions. Prior to loading, all models are relaxed using NPT ensemble (the total number of particles, the system’s volume, and the system’s pressure are constant) for 100 ps to minimize the total free energy. Then a NVT ensemble (the total number of particles, the system’s volume, and the absolute temperature are constant) is adopted to simulate the uniaxial compressive behavior by applying a constant strain rate of 0.01 ps\(^{-1}\). Young’s moduli \( E \) are calculated by the slope of the stress-strain curves (\( E = \sigma/\varepsilon \)) at a strain of 2%. All simulations are carried out at the temperature of 300 K. The time step in the MD simulations is taken as 1 fs.

Fig. 3 gives the atomic configurations at different stages. Taking the 1st group of polycrystalline DGANHCs as the example, the compressive deformation can be divided into four stages (as shown in Fig. 2b, blue line): (I) initial linear elastic stage, (II) instability of pore, (III) collapse propagation, and (IV) densification stage. At the beginning of compression, RVEs enter into the linear elastic stage. As compared to the pure ANHCs, their Young’s moduli are increased by graphene coating and the Young’s moduli of the DGANHCs are higher than those of the SGANHCs. Fig. 3(a–c) shows that, prior to reaching the peak stress, a few regions of the RVEs transform into plastic deformation from elastic deformation (Stage I). It also can be seen from Fig. 2b that the compressive strength is enhanced by the SG coating and the reinforced effect of DG coating is better than that of the SG coating. The in-plane compressive strengths of ANHCs, SGANHCs and DGANHCs are 0.70 GPa, 1.69 GPa and 2.10 GPa, respectively. The compressive strength of the DGANHCs is higher than that of the SGANHCs due to the increase in the cross-sectional area of the coating. Fig. 2b also shows...
that, compared with the critical buckling compressive strain (corresponding to the peak stress) of the SGANHCs, the reduced critical buckling compressive strain of the DGANHCs is attributed to the incoherent interface between the inner and outer graphenes which allows for free interlayer slips. This result is in contrast to the intuitive idea that the critical buckling strain could increase significantly as the coating thickness increases, but consistent with the statement that the critical axial buckling strain of a double-walled nanotube embedded in an elastic matrix is lower than that of an embedded single-walled nanotube under otherwise identical conditions reported by Ru [41]. After reaching the peak stress (i.e. the compressive strength), the pores become unstable and begin to collapse (Stage II). For the pure ANHC, the pore collapses gradually (as shown in Fig. 3d) and the in-plane compressive stress enters the plateau stage without obvious softening stage. But for the GANHCs, the graphene coatings begin to curl up and attract Al atoms to move with them under the compressive loading (as shown in Fig. 3e and f), which facilitates the collapse of the pore and results in significant softening (Stage II). Then the stress enters the plateau stage (Stage III) up to the densification stage (Stage IV). In stage IV, the strain-hardening effect becomes noticeable in the stress-strain curves,

![Fig. 1. (a, c and e) Perspective views and (b, d and f) In-plane (top) views (x-y plane) of RVEs for ANHCs, SGANHCs and DGANHCs.](image)

Table 1
Parameters of RVEs in the study.

<table>
<thead>
<tr>
<th>Group</th>
<th>Inner radii of RVEs (Å)</th>
<th>Chirality of SWCNT</th>
<th>Chirality of DWCNT</th>
<th>$\rho_{Al}^i$ of ANHC</th>
<th>$\rho_{Al}^i$ of SWCNT</th>
<th>$\rho_{Al}^i$ of DWCNT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>49.45</td>
<td>(68,68)</td>
<td>(63,63)@(68,68)</td>
<td>47%</td>
<td>13%</td>
<td>26%</td>
</tr>
<tr>
<td>2</td>
<td>46.00</td>
<td>(63,63)</td>
<td>(58,58)@(63,63)</td>
<td>54%</td>
<td>14%</td>
<td>27%</td>
</tr>
<tr>
<td>3</td>
<td>42.56</td>
<td>(58,58)</td>
<td>(53,53)@(58,58)</td>
<td>61%</td>
<td>15%</td>
<td>29%</td>
</tr>
<tr>
<td>4</td>
<td>39.12</td>
<td>(53,53)</td>
<td>(48,48)@(53,53)</td>
<td>67%</td>
<td>17%</td>
<td>32%</td>
</tr>
<tr>
<td>5</td>
<td>35.67</td>
<td>(48,48)</td>
<td>(43,43)@(48,48)</td>
<td>72%</td>
<td>18%</td>
<td>35%</td>
</tr>
<tr>
<td>6</td>
<td>32.22</td>
<td>(43,43)</td>
<td>(38,38)@(43,43)</td>
<td>77%</td>
<td>20%</td>
<td>38%</td>
</tr>
<tr>
<td>7</td>
<td>28.78</td>
<td>(38,38)</td>
<td>(33,33)@(38,38)</td>
<td>82%</td>
<td>22%</td>
<td>42%</td>
</tr>
</tbody>
</table>
as shown in Fig. 2b. The densification strain $\varepsilon_d$ is determined roughly by the point of the tangent intersection of the stress-strain curve in the densification stage with strain axis [42]. Fig. 2b shows that the densification strain $\varepsilon_d$ of the DGANHCs is lower than that of the SGANHCs, and $\varepsilon_d$ of the SGANHCs is lower than that of the ANHCs, which is mainly caused by the difference in the non-bonded Al-Al, Al-C, and C-C equilibrium distances. The non-bonded equilibrium distance is about 0.858Å, where $\sigma$ is the size parameter used in LJ 12-6 potential. As described in Section 2, the size parameters are $\sigma_{Al} = 3.407$ Å, $\sigma_{Al-C} = 3.0135$ Å, and $\sigma_{Al} = 2.62$ Å. The distance between atoms gradually decreases during densification and meanwhile the repulsion between atoms increases dramatically. That is, first the DGANHC, then the SGANHCs, and finally the ANHCs enter the densification stage. The in-plane compressive energy absorption $W$ is calculated by $W = \int_0^\varepsilon_A \sigma d\varepsilon$ and can be acquired from our MD results. Obviously, the in-plane compressive energy absorptions of the ANHCs are lower than those of the ANHCs. Yi et al. [42] reported a novel graphene-based carbon honeycomb (GCH) with giant energy absorption capacity, and they found that the GCH has a special three-dimensional structure which is different from graphene coating in the present study. The atoms along the junction line in the GCHs are relaxed into lower energy configuration with alternating distances, leading to a transition of the sp$^2$ C-C bonds along the joints into the sp$^3$ C-C bonds, which provides a high plateau stress in a longer strain range and then results in the giant energy absorption capacities of the GCHs.

Fig. 3(g–i) shows the atomic configurations of GANHCs, SGANHCs and DGANHCs, respectively, when they are fully densified. It is seen that for the ANHCs, the void can be filled by Al atoms, but for GANHCs, the gap is difficult to be filled by carbon atoms because the graphene coatings are still perfect until densification due to the strong $\sigma$ bonds between carbon atoms.

3.2. In-plane Young’s modulus

The effective Young’s modulus and yield stress of metallic foams materials have been systematically analyzed by Gibson and Ashby [7]. They derived the scaling laws correlating Young’s modulus with the relative density of the porous materials:

$$E^* = E_0 [C_1\rho^2 + C_2\rho]$$

(1)

where $E^*$ and $E_0$ are the Young’s moduli of the porous and bulk materials respectively; $\rho$ is the relative density which is defined as the mass density $\rho^*$ of the foam divided by the mass density $\rho$ of the solid material. FE analysis suggested that $C_1 = C_2 = 0.32$ [25]. Through MD simulations on indentation process of Cu monocrystals with the (0 0 1) crystallographic oriented plane, Ojos et al. [26] introduced the indenter diameter into the classical Gibson-Ashby expression to properly take into account the influence of the pore size on the Young’s modulus with the relative density of the nanoporous metal. Considering the indenter diameter is inconvenient to be used in compression tests, here the classical Gibson-Ashby expression, i.e. Eq. (1), is still applied to fit our MD results of ANHCs.

To predict the in-plane Young’s modulus $E^*$ of GANHCs, based on the classical mechanics theory for composite materials [7,43], $E^*$ can be expressed as,

$$E^* = E_0 \left[ (1 - \sqrt{1 - \rho^N}) + \frac{\sqrt{1 - \rho^N}}{1 - (1 - E_0/E^*)^2} \right]$$

(2)

where $\rho^N$ is the relative density of ANHCs, which can be seen in Table 1, and $E_0^*$ is the transverse Young’s modulus of the reinforcement phase. The values of $E_0$ of bulk monocrystal Al along [1 0 0], [1 1 1] directions and polycrystalline Al are 105 GPa, 115 GPa and 95 GPa respectively which have been evaluated through uniaxial compression tests via NVT ensemble MD simulations. For the graphene coated ANHC, we assume that $E_0^*$ in Eq. (2) equals to the radial Young’s modulus $E_0$ of the CNTs. Unlike the axial Young’s modulus $E_0$ of the CNTs, the radial Young’s modulus $E_0$ is very difficult to be determined. Reported values of the radial Young’s modulus $E_0$ vary by up to 3 orders of magnitude [44]. Yang and Li [45] measured the effective radial modulus $E_0$ of straight SWCNTs by using well-calibrated tapping mode and contact mode atomic force microscopies. It is found that the measured $E_0$ decreases from 57 GPa to 9 GPa as the diameter of the SWCNTs increases from 0.92 to 1.91 nm. Zheng et al. [46] investigated experimentally the transverse deformability of DWCNTs using an ultrathin nanomembrane covering scheme, and they reported that $E_0$ of DWCNTs decreases from 40 GPa to 6 GPa as the nanotube outer diameter increases from about 2 nm to 3.6 nm. Using the molecular structural mechanics (MSM) method, Li and Chou [47] found that the radial Young’s modulus of SWCNTs decreased from 1.3 TPa to 0.3 TPa as the diameter of SWCNTs increased from 0.5 nm to 2.5 nm. Chen et al. [48] presented a modified MSM model for determining the mechanical properties in the radial direction of SWCNTs. They found that the radial elastic modulus of the armchair SWCNTs with a radius of 0.48-2.38 nm is about 30-0.3 GPa. Wang et al. [49] used MD simulations to examine the relation between the radial compressive Young’s modulus $E_0$ of CNTs and their MD results showed that the armchair SWCNTs with a radius of 1.3-3.5 nm is about 0.65-0.03 GPa and DWCNTs with a radius of 1.2-3.7 nm is about 2.8-0.24 GPa.

Here we assume that the CNTs is a nanoporous material of graphene matrix and void, as shown in Fig. 4a and b for SWCNTs and DWCNTs respectively. Through the Eq. (1) we can calculate the Young’s modulus
of CNTs and then substitute it into Eq. (2) to get the theoretical solutions of the in-plane Young’s modulus of GANHCs. The relative density $\rho_r$ of graphenes can be calculated by $(2rt - t^2)/r^2$, where $r$ is the inner radius of RVE, and $t$ is the thickness of CNTs, whose values of SWCNTs and DWCNTs are assumed to be 3.4 Å and 6.8 Å respectively, as listed in Table 1. The $E_{\text{graphene}}$ is chosen as 669 GPa in our theoretical models, which was figured out by Reddy et al. [50] using MD simulations with Brenner’s potential.

The in-plane Young’s moduli $E^*$ of the ANHCs along the [1 0 0], [1 1 1] directions, and polycrystals with different relative densities as well as their corresponding GANHCs (i.e. groups 1–7 in Table 1) obtained from the MD simulations are listed in Fig. 5. The results estimated from the modified Gibson-Ashby approach are also shown in Fig. 5. Compared to the MD results, the classical Gibson-Ashby expression can give an accurate prediction of in-plane Young’s moduli $E^*$ of the ANHCs at a low relative density, but it becomes less accurate for a higher relative density.

As for ANHCs and GANHCs, the in-plane $E^*$ linearly increases with the increase in the relative mass density. The reinforcing effect of graphene coating on Young’s moduli can be measured by $(E_{\text{GANHC}} - E_{\text{GANHC}})/E_{\text{GANHC}}$.
$E_{\text{ANHC}}$/$E_{\text{GANHC}}$, where $E_{\text{GANHC}}$ and $E_{\text{ANHC}}$ are the in-plane Young’s moduli of GANHCs and ANHCs in case of the same group, respectively. As compared to the ANHCs with the same relative density, the Young’s moduli $E^*$ can be increased by the SG coating ranging from 52% to 177% and the DG coating ranging from 65% to 276% in [1 0 0] direction; by the SG coating ranging from 49% to 130% and the DG coating range from 64% to 197% in [1 1 1] direction; by the SG coating ranging from 72% to 163% and the DG coating ranging from 88% to 253% in polycrystals.

3.3. Compressive strength

The plateau stress for a porous metallic material is reached when its cells begin to collapse plastically. This plateau stress is often defined as the compressive strength of the porous material. For porous materials, the compressive strength can be estimated by the following Gibson-Ashby expression [7]:

$$\sigma^* = \sigma_1 \left[ C_2 \rho_1^{3/2} + C_3 \rho_1^{1/2} \right]$$

Fig. 5. Young’s moduli $E^*$ of ANHCs and GANHCs in (a) [1 0 0] direction, (b) [1 1 1] direction, and (c) polycrystalline Al.

Fig. 6. Compressive strength $\sigma^*$ of ANHCs and GANHCs in (a) [1 0 0] direction, (b) [1 1 1] direction, and (c) polycrystalline Al.
where $\sigma^*$ and $\sigma_i$ are the yield strengths of the porous and the solid cell wall materials, respectively, $C_1 = 0.33$, and $C_2 = 0.44$, which were determined by FE analysis [25]. Through MD simulations of single crystalline nanonoperous cooper under adiabatic uniaxial compression in [0 0 1] direction, Yuan and Wu [27] found that the Gibson-Ashby’s scaling law is still applicable in nanoscale, but the constants $C_1$, $C_2$ and $C_3$ in Eqs. (1) and (3) should be determined from experimental or simulation results. In this study, we will determine these four constants by fitting the MD results of ANHCs, which are listed in Fig. 6.

To get the in-plane compressive strength $\sigma^*$ of GANHCs analytically, since the radial Young’s moduli of CNTs can be analytically obtained from Eq. (1), here we assume the $\sigma^*$ of GANHCs as,

$$\sigma^* = \left[ C_2 \rho^{1/2} + C_3 \left( \rho \frac{E_f}{E_b} \right)^{1/3} \right]$$

(4)

where $\sigma_0$ of bulk Al in [1 0 0], [1 1 1] directions and polycrystalline bulk Al are 8.1 GPa, 7.4 GPa and 7.1 GPa respectively, which have been firstly determined by using uniaxial loading in an NVT ensemble. The Young’s moduli $E_f$ of bulk Al has been described in Section 3.2. $E_f$ is the radial Young’s modulus of SG coating or DG coating which can be predicted by Eq. (1) $C_2$, $C_3$ are acquired by fitting ANHC data, and $C_1$, $C_3$ are obtained by fitting SGANHC data. When Eq. (4) is used to predict the $\sigma^*$ of DGANHCs, none of any parameters are needed to fit.

For nanomaterials, surface effect may induce a size dependency in the size-independent classical elasticity theory [27,51,52], and this surface effect depends upon the crystallographic orientation [53]. Therefore, different parameters should be fitted for different crystallographic orientation. The compressive in-plane strengths $\sigma^*$ in different crystal orientations of ANHCs and GANHCs are shown in Fig. 6a–d, respectively. From Fig. 6 we can see that, the compressive strength $\sigma^*$ of GANHCs can be well predicted by Eq. (4) effectively.

The reinforced effect of graphene coatings on compressive strength can be evaluated by $(\sigma_{ANHC} - \sigma_{ANHC})/\sigma_{ANHC}$, where $\sigma_{ANHC}$ and $\sigma_{GANHC}$ are the compressive strength of ANHCs and GANHCs, respectively. In comparison to the ANHCs with the same relative density, the compressive strength $\sigma^*$ can be increased by the SG coating ranging from 38% to 110% and the DG coating ranging from 73% to 119% in [0 0 1] direction; by the SG coating ranging from 35% to 105% and the DG coating range from 83% to 146% in [1 1 1] direction; by the SG coating ranging from 48% to 128% and the DG coating ranging from 78% to 183% in polycrystals.

4. Conclusions

In summary, we have performed MD simulations and theoretical analysis to study the in-plane compressive behavior of aluminum nanohoneycombs (ANHCs) and graphene coated ANHCs (GANHCs). The compressive energy absorption capacity of GANHCs until densification is lower than that of pure ANHCs, which is mainly caused by the greater non-bonded Al-C, and C-C equilibrium distances due to the graphene coatings compared to the Al-Al equilibrium distance. It is found that the graphene coatings can significantly reinforce the tensile strength, the tensile energy absorption, the in-plane elastic modulus and compressive strength of aluminum nano-honeycombs.

In addition, we proposed a modified Gibson-Ashby model to determine the in-plane elastic modulus and compressive strength of GANHCs. For ANHCs, we found that at a low relative density, the classical Gibson-Ashby scaling laws is still applicable to predict the in-plane Young’s moduli, but as the relative density increases, the Gibson-Ashby scaling laws underestimates the values due to the stronger surface effect of the pore. Our study of the in-plane compressive strength of ANHCs shows that the constants in the classical Gibson-Ashby expression should be re-fitted from MD data and they are dependent on the loading crystal orientation. The compressive strength of GANHCs can be well predicted by the proposed expression.


