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Atomistic behavior of nanoporous carbon nanotube-aluminum composite under compressive loading

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Abstract
Metal matrix nanocomposites have been actively studied to discover the characteristics of a new class of materials. In the present study, metal matrix nanocomposites are investigated using molecular dynamics simulations of the compressive behavior of nanoporous carbon nanotube (CNT)-aluminum (Al) composites that have a density of approximately 77% to that of pure Al. The weight-reduced nanocomposites exhibited an enhanced Young’s modulus of 138%, and a compressive strength degraded by 13% compared with pure Al. Through stress decomposition into CNT and Al constituents, it was observed that the Young’s modulus was enhanced due to the high stiffness of the CNTs; further, the reduced strength was primarily due to the early failure strain. The effects of CNT volume fractions and sizes are further analyzed using the rule of mixture, which is modified by the interphase area definition. In addition, the atomistic details of the structure and stress revealed a buckling behavior in the CNT as well as a massive slip behavior in the Al matrix during plastic deformation. The results presented in this study will have implications in the design and development of metal matrix nanocomposites for applications in high-performance lightweight materials.

1. Introduction
Lightweight metal materials are essential to reduce the weight of components. This is especially true when advanced polymeric composites, which retain the enhanced strength with relatively low-density, cannot replace metals. Engineered polymeric composites have shown improved strength and stiffness; however, their poor thermal stability, low toughness, and poor electrical conductivity limit their application [1]. Thus, metals exhibiting high specific strengths such as aluminum (Al), titanium, and magnesium are still promising when low weight is critical such as in aerospace applications, automotive industries, electronic packaging, sports industries, etc [1, 2].

Metal matrix composites containing nanomaterials such as carbon nanotubes (CNTs) [3–5], boron nitride nanotubes [6–8] and graphene nanoplatelets [9–11] have been actively studied to improve mechanical properties [5, 12], to add functionality to native materials [13], or to design functionally graded materials [14, 15]. CNT-Al composites have been fabricated by several processing techniques such as melt processing, powder metallurgy, thermal spraying and electrochemical techniques [16, 17]. In experiments, they have exhibited enhanced tensile properties such as an approximately 100% increase in toughness, 130% increase in tensile strength, and 57% increase in Young’s modulus with good dispersion of CNTs [16].

Molecular dynamics (MD) simulations of CNT-Al composites have been performed to discover the mechanical behavior at an atomic level. From tensile simulations, a 31%–39% increase in Young’s moduli compared with pure Al has been observed with (4,4), (6,6), and (8,8) CNT embedded in the Al matrix [18]. From compressive tests, Silvestre et al obtained a 50 to 100% increase in the Young’s modulus of Al-CNT [19] when (6,6) CNT was inserted. The effects of defects in the CNT [20], orientations of the CNT [21], and the interfacial bonding character of Ni coatings [22] on mechanical properties have also been studied with MD simulations.
Most studies on CNT-Al composites have focused on a low volume percentage of CNTs, which is usually less than 5% volume fraction. Although the strengthening effect is significant with a low volume percentage of CNTs, the effect of weight reduction has not been utilized in previous studies. In the present work, lightweight CNT-Al composites designed with intrinsic nanopores inside large CNTs are studied using MD simulations. A series of MD simulations are performed to reveal the compressive properties of NP CNT-Al including CNT radii and the volume fraction effect. Atomistic details of the structure and stress during compression provide additional insights into mechanical behaviors of metal matrix nanocomposites.

2. Methods

2.1. Simulation setup

NP CNT-Al composites were prepared by inserting a single-walled nanotube (SWNT) into Al structure as shown in figure 1. The Al matrix structure was composed of face-centered cubic (FCC) lattice structure with a lattice constant of 4.045 Å [23]. In the first set of simulations, (19,19) CNT was inserted into an Al matrix, and Al atoms residing inside the CNT and within the van der Waals radius of the carbons were removed. The identical x and y dimensions of the simulation cell were used \( L_x = L_y \) in figure 1(a), and the cell sizes in the x- and y-directions were varied in the range of 48.6–77.0 Å to test the effect of CNT volume fraction in the range of 11.28%–27.22%. To compare the mechanical behaviors of NP CNT-Al with those of pure Al and nanoporous Al (NP Al), an additional pure Al and NP Al setup were prepared. In NP Al, a hole with a radius of 1.29 nm was drilled at the center of the pure Al. The volume fraction of the central voids in NP Al corresponded to 19%. In additional simulations, (13,13), (16,16), (24,24), and (28,28) CNTs were inserted into the Al matrix to investigate the CNT diameter effects. The x- and y- dimensions of cell size were adjusted from 44.6 to 77.0 Å according to the CNT size to reproduce a CNT volume fraction of approximately 23%–25%. The simulation systems are summarized in table 1. The \( L_z \) dimension of the simulation cell was 97.20 Å for all simulation setups. The total number of atoms ranged from 10,282 to 32,546. Periodic boundary conditions were applied in all three directions to produce bulk properties without the edge surface effects.

2.2. Interatomic potential

In the present CNT-Al system, the interatomic potentials of C–Al, Al–Al, and C–C should be defined to calculate the force acting on each atom. An embedded atom method (EAM) potential was employed for Al–Al interactions, as the EAM potential successfully represents metallic systems by introducing the embedding energy term in addition to the pairwise interaction term. The EAM potential is represented by

\[
E = F(\bar{\rho}) + \sum_{j \neq i} \phi(r_{ij})
\]

(1)

and

\[
\bar{\rho} = \sum_{i=1} \psi(r_{ij})
\]

(2)

where \( F(\bar{\rho}) \) is the embedding energy as a function of the electron density, \( \bar{\rho} \), and \( \phi(r_{ij}) \) is the pairwise potential and \( r_{ij} \) is the distance between two particles. The EAM potential functions and parameters for Al were provided.
by Mishin et al [24]. For the C-C interactions of the CNTs, the adaptive intermolecular reactive empirical bond order (AIREBO) potential was used by implementing the equation below:

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

(3)

where \( E_{ij}^{\text{REBO}} \), \( E_{ij}^{\text{LJ}} \), and \( E_{ijl}^{\text{TORSION}} \) represent covalent bonding interactions, Lennard-Jones (LJ) interactions, and torsional interactions, respectively [25]. More details can be found in the work of Stuart et al [25]. The elastic moduli of CNTs obtained with the AIREBO potential was 0.77–0.97 TPa, depending on the chirality [26], and these are in reasonable agreement with the experimental measurements of 0.9–1.7 TPa [27]. For Al-C interactions, the non-bonded LJ potential was applied using the equation below:

\[
E_{ij} = \sum_{\alpha \beta} \epsilon_{ij} \left[ \left( \frac{r_{ij}}{\sigma_{ij}} \right)^{12} - 2 \left( \frac{r_{ij}}{\sigma_{ij}} \right)^{6} \right]
\]

(4)

where \( \epsilon_{ij} \) and \( \sigma_{ij} \) are the LJ energy and distance parameters, respectively. The LJ parameters for Al-C interactions (\( \sigma_{Al-C} = 3.0135 \) Å, \( \epsilon_{Al-C} = 0.03508 \) eV) were calculated using the Lorentz-Berthelot mixing rule, with LJ parameters for Al-Al [28] and C-C interactions [29, 30].

2.3. Simulation procedure

All initial systems were equilibrated using the NPT ensemble for 100 ps prior to the compression tests. Temperature and pressure are maintained at 300 K and 0 bar, respectively, using the Nosé–Hoover algorithm [31, 32]. After the equilibrations, compression tests were performed by applying a compressive strain in the z-direction. A constant strain rate of 10 ns\(^{-1}\) was used, and the transverse stresses were maintained at zero (\( \sigma_{xx} = \sigma_{yy} = 0 \)) by adjusting the simulation cell size in the x- and y-directions. The virial stress tensor was calculated by using equation (5), which introduces the many-body potential and periodic boundary conditions [33].

\[
\sigma(r) = \frac{1}{V} \left[ \sum_{j=1}^{N} m_j v_i \otimes v_i + \sum_{n \in Z}^{N} r_n \otimes F'_n \right]
\]

(5)

where \( i \) and \( N \) are the atom index and total number of atoms, respectively, in the local cell, \( n \in Z^3 \) is a vector of three integers representing the x, y, and z offsets of the periodic images relative to the local cell, and \( F'_n \) is the partial force on atom \( i \) due to the local cell. The compression simulations were run until the strain reached 0.3. A time step of 0.5 fs was used for all simulations. A large-scale atomic/molecular massively parallel simulator (LAMMPS) was used to perform the MD simulations [34], and the simulation results were visualized using the Open Visualization Tool (OVITO) [35].

2.4. Validation of simulation procedure

The simulation procedure was validated by comparing the pure Al simulation results with the published results. The Young’s modulus of pure Al was determined to be 61.43 GPa using compression simulation, which is in close agreement with the experimentally published values of 60.2–76.1 GPa [36–38]. In addition, it is in reasonable agreement with the simulation results that reported a Young’s modulus of 64.4–74.8 GPa [11, 19, 39]. In the present study, yield stress and strain were obtained as 5.9 GPa and 0.1, respectively, which are also comparable to the published values of 6 GPa and 0.11 of yield stress and strain, respectively [19]. It should be noted that yield stress obtained by the simulation is much higher than the experimentally measured value due to

### Table 1. Summary of simulation systems.

| Model no. | Model type | CNT Vol% (%) | CNT radius (Å) | Cell size (x and y) (Å) | Relative density |
|-----------|------------|--------------|----------------|------------------------|------------------|
| 1         | Pure Al    | —            | —              | —                      | 1.00             |
| 2         | NP Al      | —            | —              | —                      | 0.81             |
| 3         | NP CNT-Al  | 24.10        | 12.88          | 52.65                  | 0.77             |
| 4         | NP CNT-Al  | 11.28        | 12.88          | 76.95                  | 0.79             |
| 5         | NP CNT-Al  | 14.10        | 12.88          | 68.85                  | 0.86             |
| 6         | NP CNT-Al  | 18.10        | 12.88          | 60.75                  | 0.83             |
| 7         | NP CNT-Al  | 23.06        | 12.88          | 44.55                  | 0.83             |
| 8         | NP CNT-Al  | 23.51        | 12.88          | 52.65                  | 0.77             |
| 9         | NP CNT-Al  | 24.10        | 12.88          | 52.65                  | 0.77             |
| 10        | NP CNT-Al  | 22.70        | 18.99          | 76.95                  | 0.79             |
a perfect lattice structure without voids, impurities, grain boundaries, and so on. A much higher strain rate used in the compression simulation may also contribute to the higher yield stress in the simulation.

3. Results and analysis

3.1. Compressive stress–strain behavior of NP CNT-Al

The stress–strain relationships of NP CNT-Al, pure Al, and NP Al under compression are first compared by plotting them in figure 2(a). It can be seen that the stress increases linearly with the strain up to a strain of approximately 0.1 in pure Al, and then the stress sharply declines to a plastic flow regime. NP Al displays similar behavior to pure Al, except that the magnitude of maximum stress and corresponding strain are different. The maximum stress of NP Al equals 4.29 GPa, which corresponds to a 17.7% reduction in stress compared with pure Al. In NP CNT-Al, the stress increases linearly up to the first stress peak point, and then the stress drops to the plastic flow regime. During the decline in stress, local stress recovery and relapse are present at the second stress peak points in the stress–strain curves. The maximum stress of NP CNT-Al was determined to be 5.13 GPa, which corresponds to a 13% reduction in stress compared with pure Al.

The Young’s moduli can be extracted from the slope of the linear elastic region. The least squares method was used for the linear region between a strain of 0 and 0.02. The calculated Young’s moduli were 146.42, 61.43, and 47.40 GPa for NP CNT-Al, pure Al, and NP Al, respectively. Note that the Young’s modulus of pure Al (61.43 GPa) is in close agreement with the experimentally measured values of 60.2–76.1 GPa [36–38]. The Young’s modulus of NP Al (47.40 GPa) is smaller than that of pure Al. However, if the stress–strain curves are corrected based on the actual area given by $A_{act} = A_{cell} - A_{pure}$, the Young’s modulus of NP Al is comparable to that of pure Al. This indicates that the reduced Young’s modulus of NP Al is due to the reduced load-supporting area.

The NP CNT-Al exhibited 58% enhancement in Young’s modulus, and a 13% reduction in ultimate compressive strength (UCS) compared with pure Al. The reduced UCS of CNT-Al composites was investigated by decomposing the composite stress into the stress of each constituent. Figure 2(b) displays the total stress of CNT-Al, and the decomposed stress for the CNT and Al matrix with the corresponding strain. As can be seen in figure 2(b), the much larger stress borne by CNT indicates that the extraordinary mechanical properties of CNT are effective. In contrast, the stress–strain curve of Al in matrix phase features degraded mechanical properties. The UCS for Al decreased from 5.9 GPa to 1.983 GPa, and the Young’s modulus decreased from 61.43 GPa to 40.76 GPa when CNT was embedded in the Al matrix. The stiffness of CNT-Al composite was higher than that of pure Al because the high stiffness of the CNT overcame the decreased stiffness of the Al matrix in the CNT-Al composite. With regards to the UCS, the decreased UCS of the Al matrix overcame the high UCS of the CNT in the CNT-Al composite. Consequently, the stiffness of the CNT-Al was higher, whereas the UCS of the CNT-Al was lower compared with pure Al.

It can be concluded that the increased stiffness of NP CNT-Al is attributable to the high stiffness of CNT, while the decreased UCS is attributable to the degraded mechanical properties of Al in matrix phase. The
decrease in the UCS of the Al matrix is mainly due to the premature failure strain. In pure Al, failure strain corresponds to a strain of approximately 0.1. In NP CNT-Al, the Al matrix fails at a strain of approximately 0.05 following CNT failure at a strain of approximately 0.04. The early failure is likely influenced by the buckling behavior of CNT, which was found at the failure strain of CNT (see figure 7). Additionally, the Young’s modulus of Al decreased in the matrix phase, which suggests that the interphase model can be used to analyze composite properties [40, 41]. In the next sections, the effects of CNT volume fraction and CNT size on mechanical properties are investigated with interphase analysis.

3.2. Effect of CNT volume fractions

The effect of CNT volume fraction on compressive stress–strain behavior and the mechanical properties of NP CNT-Al were investigated. Previous studies have reported that the size of CNT affects the mechanical strength of the Al-CNT composite [18]. Thus, to eliminate the CNT size effect, the same size of CNT, namely (19,19) CNT, was embedded in the Al matrix, and the CNT volume fractions were adjusted by increasing the simulation cell sizes. Figures 3(a)–(c) displays the stress–strain curves with varying CNT volume fractions. Total stress–strain curves are plotted in figure 3(a), and decomposed stress–strain curves for CNT and Al constituents are plotted in figures 3(b) and (c), respectively. As can be seen in figure 3(a), both stiffness and UCS increase with increasing CNT volume fractions. As the high strength and stiffness of CNT enhances the corresponding composite properties, it is clear that an increased volume fraction of CNT results in the increased stiffness and strength of NP CNT-Al. The stress–strain behaviors of (19,19) CNT embedded in different sizes of Al matrix exhibit subtle difference in the elastic regions, as seen in figure 3(b). In contrast, the stress–strain behaviors of the Al matrix exhibit a noticeable dependency of stiffness and maximum stress on CNT volume fractions, as seen in figure 3(c).

To quantitatively analyze the variation in mechanical properties with CNT volume fraction, the Young’s modulus was extracted from the linear elastic region in the strain range of 0.0–0.02 in the stress–strain curve. Figures 4(a) and (b) displays the Young’s modulus extracted from the stress–strain curves of NP CNT-Al and Al matrix, respectively. The variations are shown with the CNT volume fractions, given as \( v_{\text{CNT}} = V_{\text{CNT}} / V_{\text{total}} \). \( V_{\text{CNT}} \) and \( V_{\text{total}} \) correspond to the CNT volume and total cell volume, respectively. As discussed earlier, the Young’s modulus of NP CNT-Al increases with increasing CNT volume fractions, although the Young’s modulus of the Al matrix decreases with increasing CNT volume fractions. This indicates that the high stiffness of CNT is a dominant factor in determining the Young’s modulus of NP CNT-Al. It was demonstrated that the Young’s modulus of the Al matrix as lower when CNT was embedded than pure Al. Thus, the decreased Young’s modulus of the Al matrix with the increased CNT volume fractions can be attributed to the increased CNT interface effect, that is, the increased fraction of interphase area between CNT and Al.

The mechanical properties of composites such as the Young’s modulus, yield strength, and shear stress have been widely described by the rule of mixture (ROM). Because the strain is applied in the uniaxial CNT direction, the Young’s modulus of CNT-Al composite using ROM is written as

\[
E = E_{\text{CNT}} v_{\text{CNT}} + E_{\text{Al}} (1 - v_{\text{CNT}})
\]

\( (6) \)
where $v_{CNT}$ is the volume fraction of CNT including the CNT core hole, $E_{CNT}$ is the Young’s modulus of CNT, and $E_{Al}$ is the Young’s modulus of Al.

In substituting $E_{CNT}$ in the ROM equation, the effective Young’s modulus of the SWNT embedded in the matrix should be used. Compared with the measurement of an individual SWNT simulation, the SWNT is less stiff when it is embedded in the Al matrix. However, the reduction in stiffness does not vary with the cell size, indicating that the effective Young’s modulus of CNT does not depend on volume fraction changes if the CNT diameter and interfacial surface area remain unchanged. In contrast to $E_{CNT}$, the effective $E_{Al}$ depends on the CNT volume fraction as discussed earlier, and this dependency can be described by the interphase model. In the interphase model, the boundary region near the reinforcements have structural and mechanical properties that are different from the core region (see figure 1(b)). As the CNT volume fraction increases, the volume fraction of the interphase region also increases, and this results in a change in properties when the CNT volume fraction changes.

The ROM can be modified with the interphase area as follows:

$$E = E_{CNT}^* v_{CNT} + E_l v_l + E_{Al}(1 - v_{CNT} - v_l)$$

(7)

where $v_l$ is the volume fraction of the interphase area. $E_{CNT}^*$ is the effective Young’s modulus of CNT embedded in the matrix, which is averaged from the stress–strain curve for CNT. $E_{Al}$ is the Young’s modulus of Al, which is taken from the pure Al simulations. As the volume fraction of the interphase area is affected by the CNT size and CNT volume fraction, $v_l$ can be formulated as a function of $v_{CNT}$ and CNT radius, $R_{eff}$. From the annular geometry of the interphase area having an inner circle radius corresponding to $R_{eff}$ and an outer circle radius corresponding to $R_{eff} + d$, the interphase area is given by:

$$v_l = v_{CNT} \left\{ \left( \frac{R_{eff}}{R_{eff}^2} \right)^2 - 1 \right\}$$

(8)

where $R_{eff}$ is the effective radius for the area reinforced by CNT, given as $R_{eff} = R_c + \sigma_{C-C}/2$. $d$ is the width of the interphase area. $v_{CNT}$ is also calculated using $R_{eff}$ to determine CNT volume.

Substituting the volume fraction of the interphase areas, the modified rule of mixture (MROM) can be written as

$$E = E_{CNT}^* v_{CNT} + (E_l - E_{Al}) v_{CNT} \left\{ \left( \frac{R_{eff} + d}{R_{eff}} \right)^2 - 1 \right\} + E_{Al}$$

(9)

The Young’s modulus of the interphase Al was determined to be 42.47 GPa by defining the interphase area as having a width of $3\sigma_{Al-Al} (d = 9.05)$. Figure 4(b) compares the Young’s modulus of the Al matrix obtained from the MD simulations with the interphase model using $d = 9.045$, $E_{Al} = 61.43$ GPa, and $E_l = 42.47$ GPa. The decrease in the Young’s modulus of the Al matrix with the increase in CNT volume fraction is successfully depicted by the interphase model. In figure 4(a), the MROM for the Young’s modulus of NP CNT-Al is plotted with the MD results. The dependency of the Young’s modulus of NP CNT-Al on CNT volume fraction is well described by the proposed MROM model.

In addition, to confirm the validity of the proposed MROM and the interphase property, the Young’s modulus calculated using the MROM was compared with published results. Silvestre et al. [19] studied a CNT-Al composite with (6,6) CNT having a diameter of 0.81 nm. The volume fraction of CNT was 6.1%, and the Young’s modulus of CNT-Al was measured to be 142 GPa. Using the width and Young’s modulus of the
interphase presented in this study, the MRMO produced a Young’s modulus of 130.33 GPa for a CNT volume fraction of 6.1% and an effective radius of 0.58 nm. Choi et al [18] reported the Young’s modulus of a CNT-Al composite containing 3% volume fraction of (6,6) CNT as 99.0 GPa. The MRMO produced a Young’s modulus of 101.83 GPa for 3% volume fraction of CNT. Thus, it has been demonstrated that the MRMO with the interphase determined in the present study produced a CNT-Al Young’s modulus in reasonable agreement with the published results.

In Figure 4(c), the UCS measured as the maximum stress of the stress–strain curve of NP CNT-Al is plotted with the CNT volume fractions. As can be seen in Figure 4(c), the UCS increased with the increase in CNT volume fraction, indicating the increased strengthening effect of CNT. From the stress–strain curves, it is evident that the failure strain does not depend on the CNT volume fraction, as CNT failure determines composite failure. Thus, the variation in UCS with the CNT volume fraction can be obtained with MRMO, and is given as follows:

$$\sigma_{\text{UCS}} = [E_{\text{CNT}}^* v_{\text{CNT}} + E_{\text{f}} v_{\text{f}} + E_{\text{m}}(1 - v_{\text{CNT}} - v_{\text{f}})] \varepsilon_e$$

where $\varepsilon_e$ is the corrected strain due to the non-linearity near the maximum stress. $\varepsilon_e$ was obtained as 0.036 by fitting the measured UCS to the MRMO model. Because the stress–strain curve near the maximum point is concave, $\varepsilon_e$ is smaller than the average failure strain of 0.04. The UCS obtained using MRMO is plotted with the MD results in Figure 4(c). The MRMO model represents well the dependency of UCS on CNT volume fractions.

3.3. Effect of CNT size

The effect of CNT diameter on mechanical properties was investigated by testing different sizes of CNTs. In this test, the CNT volume fractions were set to the same values to eliminate the effect of volume fractions. Thus, the simulation cell sizes increased with the increase in CNT size. In these tests, CNT volume fraction was maintained at approximately 24%. The stress–strain curves obtained with varying CNT sizes are shown in Figures 5(a)–(c). Total stress–strain curves are plotted in Figure 5(a), and decomposed stress–strain curves for CNT and Al constituents are plotted in Figures 5(b) and (c), respectively. As can be seen in Figure 5(a), both the stiffness and strength of NP CNT-Al composites decreased with the increase in CNT radius. This behavior should be due to the CNT behavior embedded in the Al matrix. As can be seen in Figure 5(b), the stiffness and strength of CNT decreases with the increase in CNT radius.

Young’s modulus and the UCS extracted from the stress–strain curves of NP CNT-Al are shown with the CNT effective radii in Figures 6(a) and (c). The Young’s modulus of the CNT constituent extracted from the stress–strain curves of CNT is plotted with the CNT radius in Figure 6(b). As can be seen in Figure 6(b), the Young’s modulus of the CNT constituent decreases with the increase in CNT radius. Note that this behavior is in contrast to the tensile behaviors where strength and stiffness increase with the increase in CNT radii [18]. However, isolated CNT exhibited decreasing strength and stiffness with the increase in CNT radii under compressive loading [42]. The CNT constituent of NP CNT-Al appears to be in accordance with the behavior of isolated CNT under compressive loading. Using the functional form suggested by Cornwell and Wille [42], the variation in Young’s modulus with the CNT radius can be expressed as
In equation (11), the coefficients are modified for CNT embedded in the Al matrix. The coefficients are determined by fitting the MD results to equation (11), as shown in figure (b). Substituting $E_{\text{CNT}}^{*}$ into MROM, the variations in Young’s modulus and UCS with CNT radii are obtained as represented in figures 6(a) and (c), respectively. The effective Young’s modulus of the Al constituent in NP CNT-Al increases with the increase in CNT radii due to the decreasing volume fraction of interphase area. However, the variation in Al constituent is nominal compared with that of the CNT constituent. Thus, the overall behavior of NP CNT-Al with varying CNT sizes is predominantly determined by CNT behavior.

### 3.4. Atomistic details of NP CNT-Al under compression

The representative atomic structure of NP CNT-Al during the compression tests is displayed in figures 7–9. When compressive strain is applied to the NP CNT-Al, CNT demonstrates buckling behavior. Figure 7 displays the atomistic positions and corresponding stress of CNT constituents during compressive deformation. Around a strain of 0.04, the maximum compressive stress is achieved, and buckling deformation is initiated. During buckling deformation, both tensional stress (shown in red) as well as compressive stress (shown in blue) are locally imposed. Note that the range of atomic stress have been increased with the increase in strain during plastic deformation. These buckling behaviors were observed for all CNT sizes and CNT volume fractions. During plastic deformation up to a strain of 0.3, defects such as voids and cracks were not found in the CNTs.

The atomic structure and stress distribution of the Al matrix are displayed in figure 8. As can be seen in figure 8, compressive stress acts on the matrix atoms overall. However, at the boundary of CNT and Al, tensional stresses act locally due to the shear interactions between CNT and Al. Thus, the Al matrix presents reduced compressive stress at the corresponding strain compared with the pure Al structure. Furthermore, a disordered structure appears at the boundary region, which is in agreement with the interphase model used to analyze the mechanical properties of the Al matrix. During plastic deformation corresponding to $\varepsilon > 0.04$, the disordered structure and range of stress at the boundary region gradually becomes larger with increased strain.

Additionally, common neighbor analysis was performed to analyze the atomic structure of the Al matrix. The atomic structure of NP CNT-Al around the maximum stress point of matrix Al is demonstrated in figure 9(a). Most Al atoms, excluding the CNT/Al interface atoms, were found to be FCC structures. FCC structures and surface atoms at the CNT/Al interface are shown as transparent in figure 9 to disclose the inner CNT structures and HCP structures. During elastic deformation, no HCP atoms were found. However, as the strain increased, planes composed of HCP structures appeared, indicating slip plane formations. Note that the slips nucleated at the strain corresponding to the UCS. After slip plane nucleation, the Al matrix released stresses through plastic deformations. Massive parallel slip planes were found at increased strain, as demonstrated in figure 9(b). The CNT and Al matrix behavior discussed in this section were observed with all other NP CNT-Al samples prepared with different radii and volume fractions.

### 4. Conclusions

In the present study, the mechanical behaviors and properties of NP CNT-Al under compression were investigated using molecular dynamics simulations. It was observed that NP CNT-Al retained enhanced stiffness but degraded strength as compared with pure Al. Through stress decomposition into CNT and Al matrix
constituents, it was found that the increased stiffness of NP CNT-Al was attributable to the high stiffness of CNT; further, the decreased UCS was attributable to the degraded mechanical properties of Al in the matrix phase. When CNT was embedded in the Al matrix, UCS was substantially decreased due to the occurrence of failure at an earlier strain; this was induced by the buckling behavior of CNT. Additionally, the Young’s modulus of the Al matrix decreased due to the local tensional stress imposed on the interfacial Al atoms as a result of CNT-Al shear interaction.

Furthermore, the effects of CNT size and CNT volume fraction on compressive mechanical properties were investigated. Both the UCS and Young’s modulus increased with the increasing CNT volume fractions owing to the increased strengthening effect of CNT. As the CNT size increased, the Young’s modulus of CNT decreased under compression. Thus, it was found that both the UCS and Young’s modulus of NP CNT-Al decreased with the increase in CNT the radius, mainly due to the CNT behavior. The variations in Young’s modulus and UCS were illustrated using the ROM modified by the interphase area between Al and CNT. Through atomistic structure analysis, CNT buckling was noted at the strain corresponding to the UCS, and massive slip planes were
observed in the Al matrix during plastic deformation. As the present research provides a fundamental understanding of the mechanical behaviors of NP CNT-Al, including CNT size and volume fraction effects, it will be useful for designing and developing lightweight metal matrix composites containing a high volume percentage of large CNTs.

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