Behavior of the mechanical system composed of highly deformable structural elements

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Abstract. Carbon nanotubes (CNTs) are attractive for many applications because they possess a unique combination of mechanical and physical properties. Horizontally aligned CNT bundles under lateral compression behave as an elastic body with highly deformable elements, since their cross sections can collapse. Mechanical properties of such systems is poorly investigated in spite of the fact that they are promising for vibration and shock protection. Here we use a chain model with a reduced number of degrees of freedom in order to study the behaviour of a CNT bundle under uniaxial and biaxial lateral compression. Stress-strain curves are obtained and evolution of the CNT bundle structure is analyzed.

1. Introduction
Carbon nanotubes (CNTs) attract each other by non-valence interactions forming CNT bundles [1-3] that can be obtained by various experimental methods [4,5]. Individual CNTs have excellent mechanical properties, such as tensile strength from 11 to 63 GPa, Young's modulus during axial tension from 1.0 to 1.3 TPa and strain to fracture exceeding 10% [6,7]. Moreover, CNTs are lightweight, flexible, bendable, they have good thermal and electrical conductivities, that is why they can be applied in various nanotechnologies [8, 9]. CNT bundles are used to produce high-strength ropes [2, 10], fibers [11, 12], polymer and metal matrix composites [12, 13], solid lubricants [14], projectile protectors [15], etc.

Physical and mechanical properties of CNT bundles have been extensively studied with the use of computer simulation methods. Vertically aligned CNTs can be transformed into horizontally aligned forest by pressing [16,17]. The thin shell theory has been used to describe CNT ensembles of different structure [18]. In the works [19,20], the applicability of the beam, plate and shell theories to the analysis of the mechanical properties of nanomaterials has been analyzed. Importantly for the present study, CNTs having diameter above a threshold value, have two equilibrium configurations, circular and collapsed [21-23]. Mechanical properties of CNT bundles can be efficiently studied using the nonlinear coarse-grained potential [24]. In order to considerably reduce the number of degrees of freedom, the chain model has been developed for simulation of some \( sp^2 \)-carbon nanostructures [25]. In particular, this model was successfully used to study structure and properties of various conformations of carbon nanoribbons [25-29] and surface ripplocations [30]. The chain model was extended to the study of CNTs under lateral plane strain compression in [31,32]. CNT bundle as an elastic damper was analyzed in [33]. Laterally compressed CNT bundle undergoes phase transitions [34,35]. Buckling critical load for axially compressed graphene nanoribbons can be increased by
twisting about long axis [36,37]. Propagation of solitary waves and shock waves in carbon and other nanomaterials have been studied in [30,38,39].

In this work, we demonstrate the application of the chain model to the analysis of the structure evolution of CNT bundle under uniaxial and biaxial compression. In Sec. 2 we describe the model and in Sec. 3 present simulation results. Sec. 4 concludes this work.

2. Simulation method

Presented in figure 1 is a schematic representation of the computational model used in this study. The zigzag nanotubes of the same diameter are aligned with the z-axis of the Cartesian coordinate system and they create a triangular lattice in cross-section. CNTs are numbered by the two indices, \( i = 1, ..., I \) and \( j = 1, ..., J \) (\( I = J = 2 \) in the figure). The atoms move on the \((x, y)\) plane and each atom stands for a rigid row of atoms normal to the \((x, y)\) plane. Atoms within a CNT are numbered anticlockwise by the index \( n = 1, ..., N \), as shown in figure 1 for the tube with \( i = j = 1 \). Total number of carbon atoms in the computational cell is \( I \times J \times N \). Positions of the atoms are specified by the radius-vectors \( r_{ijn} = (x_{ijn}, y_{ijn}) \). We use periodic boundary conditions along directions of translation.

The equilibrium interatomic distance in graphene is \( \rho = 1.418 \text{ Å} \). In the zigzag CNT, the distance between neighbouring atomic rows parallel to the \( z \)-axis is \( a = \rho (3^{1/2})/2 = 1.228 \text{ Å} \). Diameter of CNT is \( D = a/\sin(\pi/N) \), where \( N \) is the number of atoms in the cross section of CNT. If \( d \) is the distance between neighbouring CNT walls, then the distance between centres of neighbouring CNTs is \( A = D + d \). In our simulations we take \( N = 30 \), then \( D = 11.75 \text{ Å} \) and \( d = 3.088 \text{ Å} \).

Carbon nanotube bundle in the frames of the chain model can be described by the Hamiltonian

\[ H = K + U_B + U_A + U_{vdw}, \]

where the first term in kinetic energy

\[ K = \frac{M}{2} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{n=1}^{N} \left( \frac{x_{ijn}^2}{2} + \frac{y_{ijn}^2}{2} \right), \]

the second term gives the energy of valence bonds

\[ U_B = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{n=1}^{N} V(|r_{ijn} + 1 - r_{ijn}|), \]

where \( V(r) = \frac{k}{2} (r - a)^2 \),

the third term describes the energy of valence angles

\[ U_A = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{n=1}^{N} P(\theta_{ijn}), \]

where \( P(\theta) = \varepsilon [\cos(\theta) + 1] \),

and the fourth term describes the van der Waals interactions

\[ U_{vdw} = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{n=1}^{N} \sum_{n'=1}^{N} \sum_{i'=1}^{I} \sum_{j'=1}^{J} W(|r_{ijn} - r_{i'n'}|), \]

where \( |n' - n| > 3 \) when \( i = i', j = j' \).

In Eq. (2), \( M \) is the mass of carbon atom.
According to Eq. (3), valence bonds are described by the harmonic potential with stiffness constant \( k = 25.279 \text{ eV/Å}^2 \).

In Eq. (4), the angle between valence bonds, \( r_{ijn} - r_{ijn-1} \) and \( r_{ijn+1} - r_{ijn} \), is found from

\[
\cos(\theta_{ijn}) = \frac{(r_{ijn} - r_{ijn-1} - r_{ijn+1} + r_{ijn})}{|r_{ijn} - r_{ijn-1}| |r_{ijn+1} - r_{ijn}|}.
\]

In Eq. (4) the parameter \( \varepsilon = 3.50 \text{ eV} \).

The van der Waals interactions in Eq. (5) are

\[
W(r) = \frac{\varepsilon}{6} \left[ \left( \frac{\sigma}{r} \right)^{11} - 11 \left( \frac{\sigma}{r} \right)^{5} \right],
\]

with \( \varepsilon = 0.00166 \text{ eV} \) and \( \sigma = 3.61 \text{ Å} \).

Detailed information on the chain model is given in [32,33].

3. Simulation results

In figure 2, we plot the stress-strain curves obtained for (a) compression along \( x \), (b) compression along \( y \) and (c) biaxial compression. Black (blue) line shows stress \( \sigma_{xx} (\sigma_{yy}) \) as the function of absolute value of volumetric strain \( |\theta| = (1/2) (\varepsilon_{xx} + \varepsilon_{yy}) \).

![Figure 2. Stress-strain curves for (a) compression along x, (b) compression along y, (c) biaxial compression. Black (blue) line shows stress \( \sigma_{xx} (\sigma_{yy}) \) as the function of absolute value of volumetric strain \( |\theta| = (1/2) (\varepsilon_{xx} + \varepsilon_{yy}) \).](image)

As it can be seen from figure 2, the stress-strain curves can be divided into three regions. For \( |\theta| < 0.07 \), both \( \sigma_{xx} \) and \( \sigma_{yy} \) rapidly increase with strain, and this is the first region. Within the second region, stress components show a very slow increase with strain and even a slow decrease of \( \sigma_{yy} \) can be seen in (b). Note that in (a) \( \sigma_{yy} > \sigma_{xx} \), but in (b) and (c) \( \sigma_{xx} > \sigma_{yy} \) within the second range. The second range is terminated by a sharp drop of stress components. In the third range, the stress components continue to slowly increase.

In figure 3, structure evolution of the CNT bundle is presented. The top, middle and bottom rows show the results for the compression along \( x \), along \( y \), and biaxial compression, respectively. The absolute values of volumetric strain are given for each panel. The values of strain are shown by dots on the stress-strain curves presented in figure 2.

For all modes of loading the same scenario of structure transformation is observed, reflecting the three regions observed on the stress-strain curves (see figure 2). During the first stage, crystal structure remains unchanged with slightly deformed CNT cross section, see figure 3(a), (e) and (i). In the second stage translational symmetry is still preserved but the primitive translational cells increase in size. In (b) and (c) they contain four CNTs, while in (f) and (g), as well as in (j) and (k), two CNTs. The third stage is characterised by the appearance of collapsed CNTs and the loss of crystal order. Compressive deformation during the third stage results in the increase of the fraction of collapsed CNTs.
Figure 3. Structure evolution of the CNT bundle under (a-d) compression along $x$, (e-h) compression along $y$, and (i-l) biaxial compression. Absolute value of the volumetric strain is shown for each panel.

4. Conclusions
Molecular dynamics modelling of the lateral compression of CNT bundle was performed with the use of the chain model with greatly reduced number of degrees of freedom under the assumption that the plane strain conditions are satisfied. The efficiency of the used model was demonstrated. Peculiarities of the stress-strain curves were described and linked to the structure transformation of the CNT bundle. Overall, a CNT bundle under lateral compression is an elastic material with unusual properties due to the high deformability of structural units.

In future works, the chain model can be extended for 2D materials other than graphene [40-43].

Acknowledgments
This work was supported by the State Assignment of IMSP RAS No. AAAA-A17-117041310220-8.

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