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Mechanical properties of CNT-reinforced Pt under compression: molecular dynamics simulation

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Abstract. In this study, we investigate the elastic properties of a composite consisting of platinum (Pt) and carbon nanotubes (CNTs) under the influence of an external impact using molecular dynamics simulations. The main focus of our research is on compression, and we compare the results with those obtained for a pure Pt crystal, as well as with the stretching of the composite. We employ the Modified Embedded Atom Method (MEAM) potential to describe the interaction between all particles, and we calculate mechanical stresses using the virial stress method. Our findings demonstrate that the Young's modulus of the composite is higher than that of pure platinum. Additionally, we analyze the effect of the strain rate on the elastic modulus and show that it decreases with an increase in the strain rate. Furthermore, we investigate the influence of the strain rate on the phase changes that occur in the composite. Overall, our study provides valuable insights into the elastic behavior of the Pt-CNT composite under compression and contributes to the understanding of the material's mechanical properties.
Keywords: composite, CNT, compression deformation, intense impact, molecular dynamics

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Introduction

The use of modern functional and structural materials often involves exposure to intense external forces during manufacturing or operation, which can directly impact their mechanical properties. Composites consisting of a metal matrix and low-dimensional carbon structures, such as carbon nanotubes (CNTs), have gained popularity for their potential use in various fields, including aircraft engineering, medicine, and instrumentation. These materials are

typically targeted to exhibit good corrosion resistance, high thermal conductivity, low density, and high stiffness. CNTs are particularly attractive as reinforcing elements due to their exceptional strength and rigidity [1].

Despite the rapid progress in this field, there remain several challenges associated with the production of these materials and their morphology. The most significant of these difficulties are the poor dispersion of CNTs in metal matrices and the relatively weak adhesion at the metal-CNT interface. To address these issues, it is crucial to have a more extensive understanding at the atomistic scale of the characteristics of metal-CNT interactions and their impact on the mechanical behavior of metal nanocomposites under working conditions. As is the case with polymer-based materials, achieving efficient and high-quality fabrication of metal nanocomposites requires uniform dispersion of CNTs in the matrix and the formation of a strong interfacial bond between CNTs and the metal matrix.

Researchers have focused on using a variety of metals as a matrix for composites, with aluminum alloys being one of the most widely studied materials. Various liquid-phase or solid-state methods have been attempted to disperse CNTs in an aluminum matrix [2–4]. In one study [2], it was found that the Young's modulus reached a maximum of approximately 103 GPa at a CNT content of 1.0 %, which is 41.3 % higher than that of the base material. Good CNT dispersity was found to inhibit the growth of Al grains during composite manufacturing, resulting in grain refinement hardening. The Al-CNT composite also exhibited increased hardness compared to samples without CNTs. In another study [5], ab initio simulations based on density functional theory were used to investigate the interactions between a graphene sheet and an aluminum (111) layer in C-Al NC systems with different interface configurations. Dispersion relations and electron density distributions were obtained for various interface registers, and it was concluded that the bond strength at the C-Al NC interface can be controlled by introducing a compressive in-plane strain and/or removing some atomic rows along certain crystallographic structures in the direction of the Al layer (111). Such changes improved the interfacial strength from weak C-Al secondary interaction to partially covalent bonds.

Atomistic modeling has been used extensively to analyze the properties of metal-CNT composites. With the advent of supercomputers and high-performance numerical tools, several computational methods have been developed and calibrated using experimental results to evaluate the mechanical behavior of nanocomposites. Although computational methods cannot replace experimental tests, they are widely used as ancillary tools for predicting and evaluating laboratory measurements. At the nanoscale, two main methods are commonly used: ab initio methods and molecular dynamics (MD) modeling.

Numerous publications have focused on computer modeling [6–13], where MD has been utilized to develop and test new composite nanostructures with improved interfacial adhesion and/or dispersion of nanofillers. For instance, in [15] and [16], MD was used to test new matrix designs in graphene-Al and graphene-Ni nanocomposites, respectively. In [17], nickel coating of a graphene nanofiller was tested to improve load transfer in graphene-Cu nanocomposites. In [18], MD was used to conduct an in-depth study of the interaction morphology between aluminum and graphene. To test the effect of porosity on interfacial adhesion, researchers in [19] used graphdyine as a nanofiller in Cu nanocomposites. In addition, MD can be used to study the dynamics of the crystal lattice under various types of influences. The works [20–24] consider bimetallic systems and their properties, including nonlinear excitations in the lattice, which can also occur in metal-CNT composites.

The mechanical behavior of metal-carbon nanotube (CNT) composites is of great interest in various fields, including aerospace engineering, medical applications, and instrumentation. These composites have attracted attention due to their desirable properties, such as good corrosion resistance, high thermal conductivity, low density, and high stiffness. To achieve

these properties, carbon nanotubes, owing to their exceptional strength and rigidity, are commonly used as reinforcing elements in metal nanocomposites.

However, the efficient production of such materials requires the uniform dispersion of CNTs in the metal matrix and the formation of a strong interfacial bond between CNTs and the metal matrix. This has proved to be a challenging task, as poor dispersion of CNTs in metal matrices and relatively weak adhesion at the metal-CNT interface are significant issues that need to be overcome. Thus, there is a need for extensive knowledge at an atomistic scale concerning the characteristics of metal-CNT interactions and their influence on the mechanical behavior of metal nanocomposites under workload conditions.

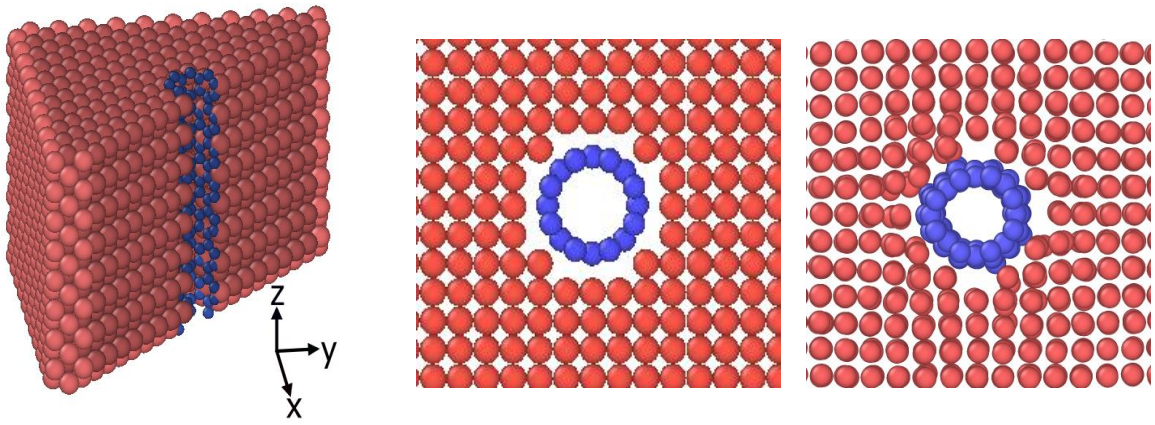
Several metals, including aluminum alloys, have been used as a metal matrix for CNT-based composites. Atomistic modeling methods, such as ab initio and molecular dynamics (MD) simulations, have been widely used to predict and evaluate the mechanical behavior of these composites. However, most of the studies conducted to date have mainly focused on the behavior of metal-CNT composites under tension. The behavior of these composites under compression has been studied much less, despite the fact that nanocomposites used in devices and systems can be subjected to both tension and compression.

In this work, we report a study of the mechanical behavior of a platinum-carbon nanotube (Pt-CNT) composite under compression. The choice of platinum as a metal matrix was based on its unique properties, such as excellent catalytic properties, and its potential use in medicine and electronics. The study of the behavior of CNT-metal composites under compression is particularly important, as CNTs under compression can be susceptible to warping and kinking, which can affect the overall mechanical properties of the composite.

Model and experimental technique

The construction of the model involved several steps. Firstly, a single-crystal platinum (Pt) structure was created, consisting of a face-centered cubic lattice with a lattice constant a = 3.920 Å. The crystal was shaped into a cube with an edge size of 43.1541 Å, and contained 5324 atoms oriented along the x - <100>, y - <010>, and z - <001> crystallographic indices.

To simulate the Pt-CNT nanocomposite, a cylindrical hole with a diameter of D = 8.4 Å was created along the z-axis of the single-crystal metal prism. All metal atoms within this cylindrical space were then removed (refer to Fig. 1(a)). A single-layer carbon nanotube of the "zigzag" type with chiral indices (8.0) was inserted into the hole, with a length of L = 43.15 Å, diameter of D = 5.2 Å, and containing 320 atoms (referred to as N). This resulted in a volume fraction of CNTs in the Pt-CNT composite of 5.8 %. All structural manipulations were performed using the Atomsk software program [25].



(a) (b) ©

Fig. 1. Fragment of a model of a Pt crystal reinforced with CNTs: (a) three-dimensional sectional view, (b) before system relaxation, (c) after system relaxation

The modeling of the deforming load was carried out by the molecular dynamics method in the LAMMPS software package [26]. It has all the functionality necessary for this work for modeling and subsequent analysis of the nanocomposite deformation. The MEAM potential was chosen to describe the interaction between Pt-Pt, C-C, and Pt-CNT. The interatomic potential of the Pt-CNT system in the considered composite was developed based on the formalism of the second modified nested atom nearest neighbor method (2NN MEAM) [27]. Visualization of the calculation results and their graphical representation for further analysis was carried out using OVITO [28].

To initiate the deformation process, the model underwent an additional relaxation for 1 ns in the NPT ensemble with periodic boundary conditions at a temperature of T = 300 K and zero pressure. This allowed for the minimization of residual stresses and free volume within the crystal. Figure 1(c) illustrates an example of a Pt-CNT composite model after the primary relaxation process.

During the compression simulation, the composite was loaded along the z-axis at a strain rate ranging from 10^{-7}–10^{-9} ps^{-1}. This strain rate was deliberately chosen to strike a balance between computational speed and accuracy. To simulate uniaxial compression of the composite, the NVT ensemble was employed at a temperature of 300 K, and the time step was reduced to 0.5 fs.

Mechanical stresses were calculated using the virial stress approach, as follows: the deformation process began with additional relaxation of the model for 1 ns in the NPT ensemble with periodic boundary conditions at a temperature of T = 300 K and zero pressure. This made it possible to minimize residual stresses and free volume in the crystal. Figure 1(c) shows an example of a Pt-CNT composite model after primary relaxation.

During compression simulation, the composite was loaded in the direction of the z-axis with a strain rate of 10^{-7}–10^{-9} ps^{-1}, which is lower than the typical strain rate used in other similar models [29,30]. This was carried out purposefully in order to reach a compromise between speed and counting accuracy. When simulating uniaxial compression of the composite, the NVT ensemble was used for a temperature of 300 K. The time step was reduced to 0.5 fs.

Mechanical stresses are calculated from the virial stress as follows:

$$\sigma(r) = \frac{1}{\Omega}\sum_i \left[-m_i \dot{U}_i \times \dot{U}_i + \frac{1}{2}\sum_{i \neq j} r_{ij} \times f_{ij}\right], \quad (1)$$

where Ω — overall volume; m_i – mass of an atom i; u_i — derivative with respect to time, which refers to the displacement vector of atom i with respect to the initial position; r_{ij} – the distance between the position vectors r_i and r_j of atoms i and j, respectively; f_{ij} – interatomic force acting on the atom i from the atom j [31]. The compression simulation was performed until the strain ε reached a value of -0.3.

Results and discussions

At the first stage of analysis, the effect of compression strain rate on the main characteristics of the Pt-CNT composite was examined, including changes in energy (E, eV), stress (σ, GPa), and Young's modulus during deformation. Figure 2 displays the change in potential energy as a function of deformation.

An increase in potential energy due to compressive load is depicted in Fig. 2. It can be observed that the curves for all strain rates have a parabolic (quadratic) shape. Notably, the dependence is almost indistinguishable among the strain rates, and the strain rate does not fundamentally affect it. A comparison with the dependence for pure Pt at a rate of 10^{-9}/ps is also shown. It is evident that the composite has a slightly higher binding energy per atom than the pure metal.

Figure 3 presents the stress-strain curve at various speeds under compressive load. The initial stress stage increases almost linearly up to 15 % regardless of the compression rate.

In this section, Hooke's law and the elastic component of deformation can be discussed. Furthermore, at higher compression rates, a decrease is observed, which may be due to the possible shortening of atomic bonds at the metal–CNT interface. The jumps observed in the range of 0.15-0.23 ε indicate some phase changes in the material, which are affected by the strain rate. As the compression speed decreases, the phase transition shifts towards larger deformations. Notably, a pronounced jump in strength is not detected for pure platinum.

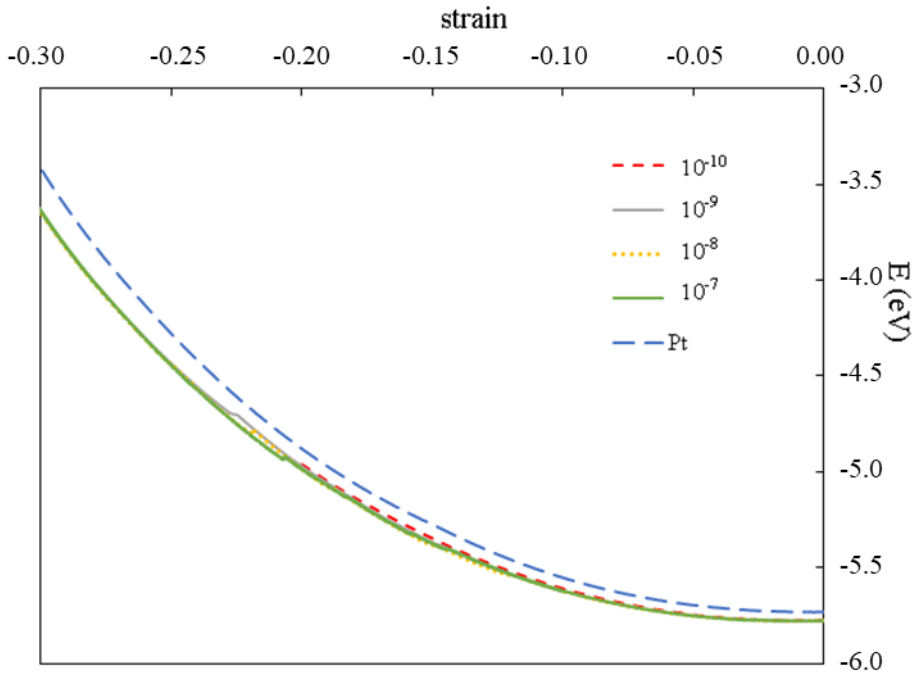


Fig. 2. Change in potential energy for pure platinum and Pt-CNT under compression for various speeds

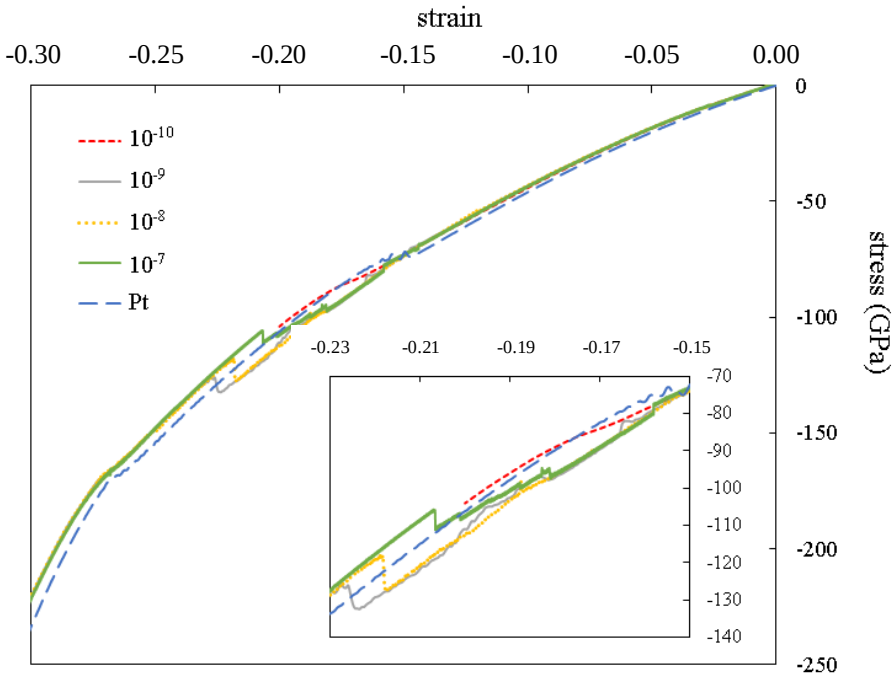


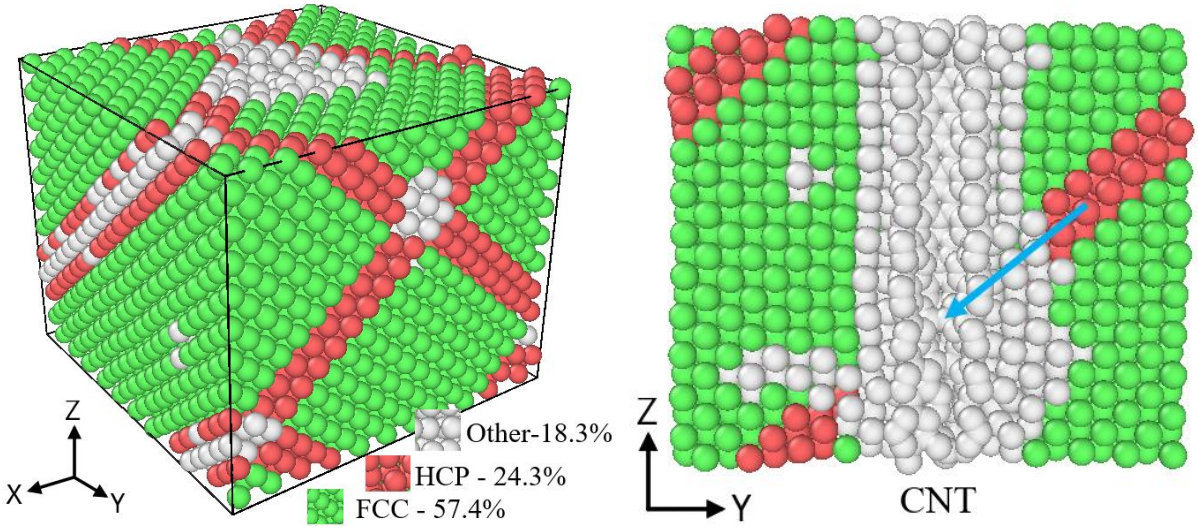
Fig. 3. Stress/strain at speeds (10^{-10}, 10^{-9}, 10^{-8}, 10^{-7})/ps under compression

Young's moduli for the considered cases of strain rates were calculated using regression analysis. Table 1 shows the results of calculating the Young's Modulus under uniaxial compression of the Pt-CNT composite at various strain rates.

Table 1. Young's modulus of Pt-CNT at various strain rates

Strain rate, ps^{-1}	Young's modulus (*E*), GPa
10^{-7}	496.1
10^{-8}	494.0
10^{-9}	561.5
10^{-10}	480.3

Through uniaxial compression testing, it was determined that the inclusion of carbon nanotubes (CNTs) in a platinum crystal resulted in an increase in Young's modulus, with the maximum increase observed at a compression rate of 10^{-9}/ps. However, the Pt-CNT nanocomposite exhibited lower elasticity compared to pure platinum. This decrease in reversible strain ability can be attributed to the introduction of additional mechanisms of deformation energy dissipation associated with the inclusion of carbon nanotubes. This observation suggests that introducing CNTs to the metal matrix can lead to the emergence of new properties, including the damping feature observed for CNT arrays (as reported in previous studies [32–33]). In further support of this theory, the compressional strain of a CNT bundle was studied in [34–38].



(a) (b)

Fig. 4. Defect structure at speed 10^{-9}/ps under compression: (a) dislocation grid at 35 % strain; (b) mechanism of CNT destruction during dislocation glide

The mechanism of formation of certain mechanical properties is largely associated with the dislocation structure of the crystal. In Figure 4(a), one can observe the dislocation network obtained as a result of deformation. An increase in deformation leads to the motions of atoms and the destruction of the CNT structure. In Figure 4(b), the arrow shows the direction of such movement and the destruction of the nanotube.

The results showed that, in addition to changes in interatomic distance, the shape evolution of the nanotube can act as a channel for energy dissipation, thus decreasing the total deformation of the composite. Overall, the findings suggest that the inclusion of CNTs in metal matrices has the potential to lead to the development of new composite materials with unique properties, which could be useful in a wide range of applications.

Conclusion

The present study investigates the behavior of a Pt-CNT nanocomposite, where the atoms interact through the MEAM potential, under uniaxial compression using the molecular dynamics method. The effect of compression rate on the binding energy, Young's modulus, and elastic stress is analyzed. Our findings demonstrate an increase in the Young's modulus of the Pt-CNT composite compared to pure platinum when subjected to compressive loading. Furthermore, we observe a decrease in the modulus of elasticity with an increase in the strain rate. Additionally, our results suggest that the compressive strain rate plays a critical role in determining the phase changes in the nanocomposite. Overall, the present work provides insights into the mechanical properties of Pt-CNT nanocomposites and highlights the importance of strain rate in determining their behavior under compression.

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