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Tensile mechanical characteristics and deformation mechanism of metal-graphene nanolayered composites

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ABSTRACT

Metal-graphene nanolayered composites (MGNLCs), composed of alternating layers of metal (copper here) and graphene layers, are new emerging engineering materials with outstandingly enhanced mechanical properties thanks to the high intrinsic in-plane strength and modulus of one-atom-thick layers of graphene. In this paper, mechanical behavior and elastic-plastic deformation mechanisms of MGNLCs subjected to uniaxial tensile loading were investigated based on molecular dynamics (MD) simulations. Stress-strain curves of the composite samples and their elastic properties were obtained and compared with their pure metal counterparts. In addition, influence of thickness of the metal layers on the composite performance was determined which seems tough or even impossible to be dealt with by the experimental techniques. Graphene inclusion outstandingly increased strength and failure strain of the composites and remarkably improved their stiffness and toughness. Graphene layers could provide effective barriers against shearing flows and dislocation propagation of the metal layers and made the applied strain energy spread out more evenly inside the material.

1. Introduction

In addition to the nanotubes, graphene which is ever known as the strongest material in the world [1] (it is about 200 times stronger than the strongest steel) has been utilized to strengthen different basic materials such as polymers, glasses, ceramic, and metals in recent years [1–5]. Metal-graphene nanolayered composites (MGNLC) are recently developed engineering materials in which alternating layers of metals and graphene sheets have been combined in order to achieve new metal-based composites with considerably enhanced mechanical characteristics [3,5–13]. For the first time, Kim et al. [6] reported the development of MGNLCs with remarkably improved properties by employing monolayer graphene sheets as a strong enhancer. They utilized nanopillar compression test to examine the mechanical properties of the synthesized MGNLCs. Their results demonstrated a considerable enhancement in the strengths of Ni- and Cu-graphene multilayers due to the effective constraint on dislocation propagation across the metal-graphene interface. Rezaei et al. [4] showed by MD simulations that the monolayers of graphene could effectively enhance the ductility and toughness of metallic glasses by providing an impermeable barrier on the propagation path of shear bands. Liu et al. [9] utilized molecular dynamics (MD) simulations to investigate effect of graphene inclusion on shock strengthening of MGNLCs for Ni and Cu metals. Their results revealed that the graphene layers could improve the shock strength of the composites. The intrinsic strong in-plane strength of the graphene as a single-atomic-layer material could provide effective barrier across the propagation path of the dislocation formed in the metal layers. Rezaei et al. [5] investigated compressive behavior of MGNLCs by utilizing MD simulations. According to their obtained results, the graphene inclusion outstandingly influenced the deformation mechanism of the composite materials by converting it from dislocation propagation to deformation twinning. However, the literature review indicates that there exists a very limited number of published work regarding the nanolayered composites. Hence, their mechanical characteristics and deformation mechanisms especially with metal layers of thickness reduced to a few atoms have not been yet delineated from the previously published studies.

The purpose of the present study was therefore to investigate the mechanical behavior and elastic-plastic deformation of MGNLCs subjected to tensile loading for FCC (face centered cubic) metal based matrix by employing MD simulations. Their elastic properties were then obtained based on elastic regions of stress-strain curves. In addition, dependency of the nanolayered composites to thickness of the metal layers was also determined. To do this, various nanolayered samples composed of alternating graphene and layers of Cu metal of different thickness were constructed and exposed to uniaxial tensile loading.

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2. Methodology

2.1. Interatomic potentials

Embedded atom method (EAM) potential [14,15] was employed to describe the atomic interactions of the Cu atoms inside the matrix. Tersoff potential function [16,17] was used to represent the covalent bonds of the C atoms of each individual graphene layer. The interfacial interactions between the metal and graphene layers and also between the graphene layers were represented by 12-6 Lennard-Jones (LJ) potential functions. LJ energy functions, as a common approach, have been widely used by the researchers to describe the weak nonbonded interactions of van der Walls type between the nanostructured reinforcements (including nanotubes and graphene) and matrix particles in the nanocomposites modelled by MD simulation technique [6,9,18–23]. For instance, Choi et al. [23] utilized the 12-6 LJ function to define the interface of nanotube and aluminum matrix. According to those available in the literature for Cu [24] and C [25] atoms, the LJ potential parameters were then calculated for Cu-C interactions based on Lorentz-Berthelot mixing rule. A more detailed description of the potential function and its corresponding parameters can be found in the previous publication of the author and coworkers [2]. The total potential energy of the composite were then obtained by adding the aforementioned functions as

$$E_{\text{total}} = E_{\text{eam}} + E_{\text{Tersoff}} + E_{LJ}^{\text{C–C}} + E_{LJ}^{\text{C–Cu}} \quad (1)$$

where E_{eam} and E_{Tersoff} represents the EAM and Tersoff potentials of the matrix and reinforcement, respectively. $E_{LJ}^{\text{C–C}}$ and $E_{LJ}^{\text{C–Cu}}$ stand for the van der Walls interactions of carbon and copper atoms between the metal and graphene layers.

2.2. Simulation setup

In order to examine the mechanical response of MGNLCs and compare them with pure metal matrix, various pure metal and nanolayered samples of different thicknesses were constructed. The pure metal samples were made of pure crystalline Cu atoms arranged in an FCC crystalline structure. The nanolayered samples as implied from their name are composed of alternating nano-layers of FCC metal and graphene. The constituting layers of the composites started at bottom and also ended at top by a metal layer, which are embedding the graphene layers as shown in the schematic diagrams of Fig. 1. Fig. 1(a) shows the atomic configurations of pure Cu samples of dimensions 20, 10, and p (nm) along the coordinate axes x, y, and z, respectively, perpendicular to the crystalline planes $(1\,\bar{1}\,0)$, $(1\,1\,\bar{2})$, and $(1\,1\,1)$. Fig. 1(b) shows the configurations of the MGNLC samples comprised of three layers of graphene and four layers of FCC structures of Cu atoms for which same crystalline directions were employed as pure samples in Fig. 1(a). An illustrated sample of the constructed nanolayered composites prepared for the MD simulations has been shown in Fig. 1(c). The left inset demonstrates the atomic structure of Cu layer with the above-mentioned crystalline directions and the right one illustrates zigzag honeycomb network of the graphene layers. In order to investigate impact of thickness, four different composite samples of the total thickness p= 10.2, 6.9, 3.6, and 1.9 (nm) were constructed in which the numbers of (1 1 1) crystalline planes of Cu atoms were 11, 7, 3, and 1, respectively. Hereafter, they are denoted by C1, C2, C3, and C4 and their corresponding pure metal samples by P1, P2, P3, and P4, respectively. Their carbon atomic fractions were 12.8, 18.7, 35, and 61.7 at.%, respectively. Boundary conditions of the both metal and nanolayered samples were assumed periodic in both x and y directions and free in z direction. The publically available MD simulation package LAMMPS ((Large-scale Atomic/Molecular Massively Parallel Simulator) was employed to perform all the simulations [26]. OVITO package was also utilized to visualize atomic structures of all the samples [27].

All the samples were first equilibrated under an isothermal-isobaric (NPT) ensemble and then loaded along the x axis under a canonical (NVT) ensemble. The time step of 0.001 (ps) was used to integrate the equations of motion based on velocity-Verlet time integrator. The tensile strain rate of 0.0001 (1/ps) was utilized to load the samples at the constant temperature of 300 K. It was adopted according to the size of the test samples and the available computation capacity on the one hand and having sufficient accuracy in the results on the other hand. To determine possible dependency to strain rate and to confirm the conducted simulations, various strain rates including 0.00005, 0.0002, 0.0005, and 0.001 (ps) were applied and compared to the main rate 0.0001. Table 1 shows the calculated elastic properties (Young's modulus E_x and Poisson's ratio ν_{xy}), for example, of sample C1 by different loading rates. It was observed that the mechanical responses of the samples were almost independent of the loading rate especially for the elastic regime. The supplementary material Fig. S1 shows the obtained stress-strain curves of the sample for the employed strain rates.

3. Results and discussion

After relaxing all the pure and composite samples under an NPT ensemble via a 58 ps-duration equilibration process, they were then stretched by applying uniaxial tensile loads along the length axis x. In the following, mechanical behaviors of all the pure and composites samples will be discussed based on extracted stress curves from MD atomic analysis versus externally applied strain. Then elastic properties of the nanolayered composites derived from elastic regions of strass-strain curves are shown and compared with their counterpart pure ones. Lastly, deformation mechanisms of all the samples under the applied loadings will be illustrated at different strains on the basis of atomic strain.

3.1. Stress-strain curves

Fig. 2(a) shows the stress-strain curves for all the pure metal nanosamples of different thicknesses P1, P2, P3, and P4 exposed to uniaxial tensile loading in comparison to each other. The samples first stretched in an elastic manner under the applied loading, then experienced yielding by reaching the maximum stress and deformed plastically after that. As can be seen, the influence of thickness on the metal behavior was not considerable. In other words, the sample size in the z direction left no noticeable effects on their mechanical responses to the applied loads at least in the considered rage. To confirm this conclusion with more confidence, a thicker metal sample of total thickness p= 13.6 (nm) (labeled as P0) was constructed, equilibrated and then exposed to same boundary and loading conditions. A similar mechanical response was observed for P0. The supplementary material Fig. S2 shows stress curve of P0 versus strain in comparison to other pure samples.

Fig. 2(b) shows the tensile stress-strain curves of all the MGNLC samples C1, C2, C3 and C4 in comparison to each other. They first deformed in an elastic manner under the applied load. By increasing the load, the metal layers experienced yielding at the first small drop observed on the stress curves (indicated by A on Fig. 3) which occurred at a strain less than that of the pure sample. This reduction in the yielding strain can be attributed to the impact of Cu-C mutual interactions at the metal-graphene interfaces and therefore to the load transformation through them. In addition, the three graphene layers divided the pure matrix to four metal layers with thickness (p) less than one-fourth of the total thickness (p).

The nanolayered samples could stand out against the applied load until the first big drop in the stress curves (marked by B on Fig. 3) where one of the graphene layers broke. Then the two other graphene layers successively (points C and D on Fig. 3) and therefore the composites failed by increasing the tension load. As observed the graphene inclusion significantly increased the strength and failure strain of the nanolayered samples. By reducing the thickness of metal layers from C1 to C4, the strengthening effects of the graphene layers outstandingly