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Effects of chirality and number of graphene layers on the mechanical properties of graphene-embedded copper nanocomposites

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ABSTRACT

In this paper, the mechanical properties of a single-crystal copper nanosheet and graphene nanoribbon-embedded copper (GNR/Cu) nanocomposites are investigated using the molecular dynamics (MD) method. Five different simulation models are used to investigate the effects of chirality, number of graphene layers, and temperature on the mechanical properties of GNR/Cu nanocomposites. The results show that the Young's modulus, tensile strength, and fracture strain of GNR/Cu nanocomposites are much larger than those of a single-crystal copper nanosheet. For the GNR/Cu nanocomposites, the number of graphene layers has a large effect on the Young's modulus and tensile strength. Conversely, the chirality influences the tensile strength and fracture strain the most, but has little effect on the Young's modulus. With increasing temperature, the mechanical properties of both the single-crystal copper nanosheet and the GNR/Cu nanocomposites deteriorate.

0. Introduction

The single-layer graphene sheet is a one-atom-thick two-dimensional layer of carbon that was discovered and successfully isolated from bulk graphite by Novoselov et al. [1]. Much research has been performed to investigate the electronic and mechanical properties of graphene, and theoretical studies and experiments have both indicated that the single graphene sheet has unusual mechanical properties and thermal conductivity [2–5]. Its unique properties of mechanical strength (Young's modulus $Y = 1.0$ TPa) [6] and thermal conductivity ($\sim$4840–5300 W m^{-1} K^{-1}) [7] have attracted significant interest for next-generation nanocomposites, such as the next generation of polymer [8–10] and metal matrix composites [11]. Additionally, extensive studies have also shown that graphene is an ideal material for thermal devices [12,13]. At present, metals are widely used as a matrix material for composites [14–16]. One possible way to apply the excellent properties of graphene would be to incorporate graphene sheets in a composite material.

Nanocomposites are a type of multi-phase solid material where at least one of the phase dimensions is less than 100 nm, or the structure has nanoscale dimensions [17]. This definition of a nanocomposite includes many types of materials, such as metals, polymers, ceramic materials, and porous media. The excellent mechanical properties of the graphene sheet makes it suitable as reinforcing fibers in polymer-, ceramic- and metal-matrix super-strong composites [18–23]. In instance, Wang et al. explored a novel methodology to fabricate bulk graphene aluminum composites based on flake powder metallurgy and the mechanical properties of composites were tested [20]. The thermal conductivity of the graphene/nickel composites is about 15% more than that of pure nickel electrodeposits [22]. The graphene flakes can be effective nanofillers of copper composites and dramatically enhanced the mechanical properties of graphene/Cu composites [23]. Because of the effect of graphene, these nanocomposites exhibited enhanced mechanical characteristics.

In the present work, the mechanical properties of armchair graphene nanoribbon (AGNR) and zigzag graphene nanoribbon (ZGNR) copper nanocomposite materials are investigated. Five models are considered: single-layer AGNR copper (SAGNR/Cu), double-layer AGNR copper (DAGNR/Cu), single-layer ZGNR copper (SZGNR/Cu), double-layer ZGNR copper (DZGNR/Cu), and a single-crystal copper nanosheet. All of these models are investigated under uniaxial tension using molecular dynamics (MD) simulations. Different temperatures are considered, and the mechanical

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properties of the graphene nanoribbon-embedded copper (GNR/Cu) nanocomposites and a single-crystal copper nanosheet are determined and discussed.

1. Method and models

Five different simulation models were used in this study. As shown in Fig. 1, these models included a perfect single-crystal copper nanosheet, a SAGNR/Cu nanocomposite, a DAGNR/Cu nanocomposite, a SZGNR/Cu nanocomposite, and a DZGNR/Cu nanocomposite. The lattice directions of [100], [010], and [001] is along the *x*, *y*, and *z* coordinate axes, respectively [24]. The crystallographic orientation of Cu nanosheet is ⟨100⟩. The AGNR/Cu nanocomposite sample had an armchair graphene nanoribbon embedded between two copper matrices along the *z*-axis, that is, the [001] direction. The ZGNR/Cu nanocomposite was defined in the same way as the AGNR/Cu nanocomposite except for the change in graphene chirality. The dimensions of the square cross-section areas were about 28.9×28.9 Å^2 for both the single-crystal copper nanosheet and GNR/Cu nanocomposites. The lengths of all of the models were set to 50 Å to avoid the influence of length on the simulation results. For all of the simulations, no periodic boundary conditions were applied. The AIREBO potential has been used to describe the interaction between the carbon atoms and the cut off distance was set to 1.95 Å to avoid the unphysically high fracture stresses. Prior to the MD calculations, the single-crystal copper nanosheet and the GNR/Cu nanocomposite systems were relaxed to make sure that the system is in equilibrium by using the Nosé–Hoover pressure barostat under the conditions of constant pressure and temperature (NPT) integration [25]. Thereafter, the system was stretched uniformly along the *z* direction at a constant strain rate in the constant volume and temperature (NVT). The temperature was kept constant at 1, 100, 300 K, respectively. That is, three simulations were performed for the single crystal copper nanosheet and each GNR nanocomposite. Then, the uniaxial tensile strain loading was applied in the stretching end along the *z*-direction with a strain loading rate of 0.00032 ps^{-1}. The simulation time step is 0.5 fs. After every step of stretching, a relaxation time 10 ps after each stretching distance 0.08 Å was applied to ensure the simulation system has enough time to relax. The LAMMPS MD program package was used to perform the simulations [26].

The interactions between the atoms in the single-crystal copper nanosheet were described by the embedded-atom method [27–29]. The total energy of the single-crystal copper nanosheet system can be described as

$$E_{Cu} = \sum_i F(\rho_i) + \frac{1}{2}\sum_{\substack{i,j \\ i \neq j}} \varphi_{ij}(R_{ij}), \tag{1}$$

$$\rho_i = \sum_{i \neq j} f(r_{ij}), \tag{2}$$

where E represents the total energy of the copper system, φ_{ij} is the two-body central potential, R_{ij} is the distance between different atoms i and j, $F(\rho_i)$ is the embedded energy, and ρ_i is the electron cloud density of the i th atom.

For the graphene nanoribbons, a second-generation reactive empirical bond-order potential was used to describe the C–C bonding interactions [30]. The potential function is given by

$$E_{GNR} = \sum_i \sum_{j(>i)} [V^R(r_{ij}) - b_{ij} V^A(r_{ij})], \tag{3}$$

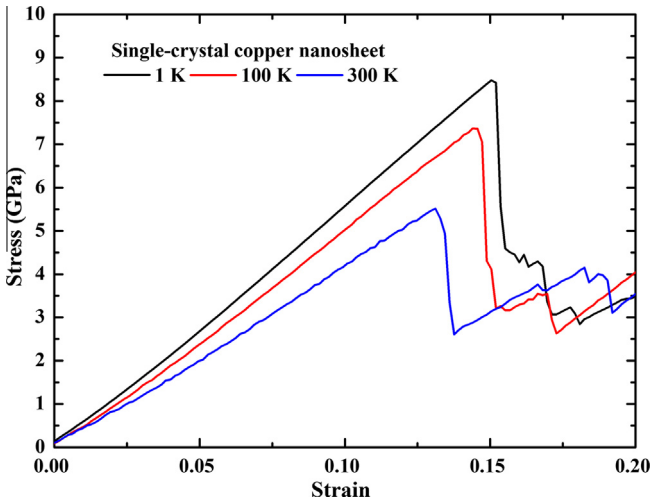

Fig. 2. Stress–strain curves of the single-crystal copper nanosheet at various temperatures.

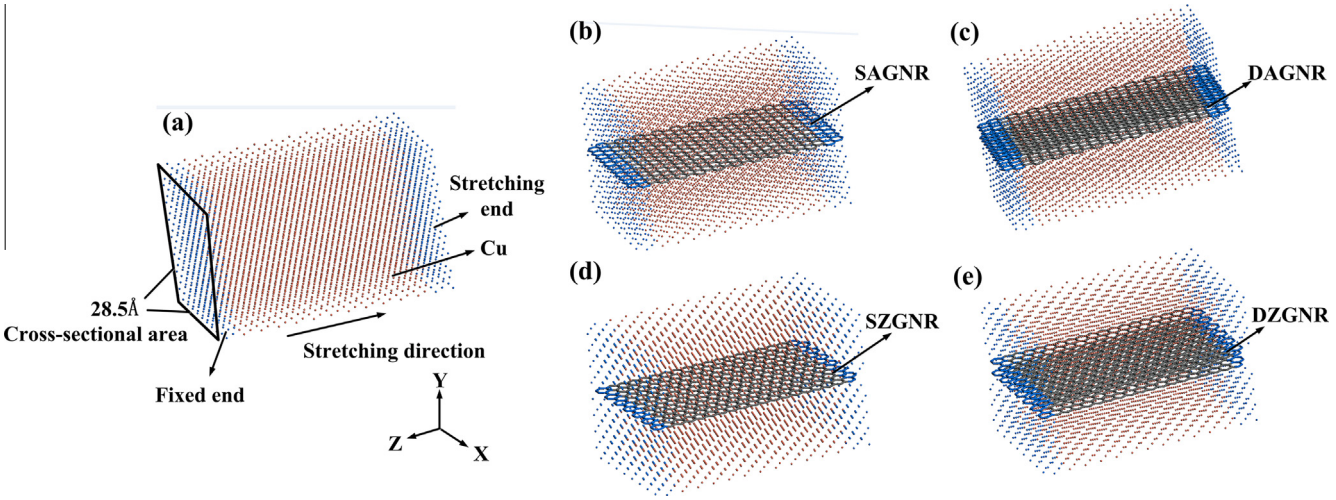

Fig. 1. Simulation models for the (a) single-crystal copper nanosheet, (b) SAGNR/Cu nanocomposite, (c) DAGNR/Cu nanocomposite, (d) SZGNR/Cu nanocomposite and (e) DZGNR/Cu nanocomposite.