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Molecular dynamics studies on the strengthening mechanism of Al matrix composites reinforced by grapnene nanoplatelets

Y. Rong, H.P. He*, L. Zhang*, N. Li, Y.C. Zhu

Department of Engineering Mechanics, Zhengzhou University, Zhengzhou, China

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ABSTRACT

Graphene nanoplatelets (GNPs) have been widely used, to strengthen different types of materials including polymers, ceramics, and metals due to their extraordinarily high strength. In this work, we, investigated the influence of GNPs on the mechanical characteristics of, GNP/Al composites by using molecular dynamics simulations. Four different, molecular dynamics models with varying GNP geometry size and charity are, established to study the deformation and strengthening mechanism of, GNP/Al composites. The simulations provide insights into various fracture, behaviors at the atomic scale, including lattice disordering, local, changes in lattice structures due to stacking faults. The results reveal, that the addition of a small amount of GNPs led to a significant, enhancement in stiffness and strength of GNP/Al composites. It further, reveals that the elasticity and strength enhancement is proportional to, GNP Size. In addition, the GNP/Al composites reinforced by armchair GNPs, show better enhancement in the mechanical behavior of reinforced matrix, than those strengthened by zigzag GNPs. It also reveals that the fracture, behavior of GNP/Al composites is mainly governed by GNPs.

1. Introduction

Al matrix composites have been extensively applied in aviation, aircraft and automobile industries because of its low density, high stiffness, superior mechanical properties, good corrosion resistance, excellent thermal conductivity and easy forming processing [1–3]. In recent years, due to the gradual development of technology and the advantages of nanomaterials, nanofillers have gradually entered the eyes of researchers. There have been reports on improving nanomaterials performance by adding nanofillers, such as carbon nanotubes and graphene [4–5].

Graphene has attracted the attention of scientists in the fields of physics, chemistry and materials because of its unique two-dimensional structure and many excellent properties. As a new material, adding a small amount of graphene can greatly improve the properties of the composite, so it can be used as an ideal reinforcement [6–9].

Bartolucci et al. [10] prepared graphene and Al composites by combining physical grinding and hot isostatic pressing. The mechanical properties and microstructure of the composites were characterized and the influence of the morphology of graphene on the strength of Al matrix composites was studied.

Wang et al. [11] successfully prepared graphene/Al composites based on flake powder metallurgy, and realized the uniform distribution of graphene in the Al matrix. Compared with pure Al, the tensile strength can be increased by 62% to 249 MPa.

Bustamante et al. [12] prepared graphene evenly distributed graphene Al matrix composites by changing the milling time and the amount of Graphene nanoplatelets (GNPs). They eventually found out that the hardness of the composite relative to Al matrix improved 138% with the graphene content of l.0 wt%.

Li et al. [13] used the composite process of cryogenic ball milling and hot extrusion to prepare graphene reinforced Al matrix composites, and investigated the effects of graphene addition on microstructure and mechanical properties of the composites. The experimental results show that the tensile strength and yield strength of the composites are increased compared with that of pure Al and the elongation of composite material doesn't decrease with the addition of graphene.

Rashad et al. [14–15] used ultrasonic agitation to deal with graphene powder, to ensure its distribution more evenly in the alloy matrix. Then, Al base alloy is finally obtained by powder metallurgy forming, sintering and subsequent hot extrusion. It is found that the strength of the composite is enhanced obviously, and the enhancement effect of graphene is better.

However, due to the uneven dispersion of graphene in the dispersion process, it is easy to agglomerate, so the graphene content in the composite material is low, this leads to that even graphene has many unique properties, but it cannot be fully utilized. Although there have already started the research of graphene Al matrix composites, but the

* Corresponding authors.
E-mail addresses: hehuiping@zzu.edu.cn (H.P. He), ielzhang@zzu.edu.cn (L. Zhang).

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research has just started, on graphene dispersion of graphene in the Al matrix, and graphene substrate wettability, and interface control problem is far from solved completely, coupled with the high cost of raw materials and the preparation process of graphene composites cost, restrict the use and promotion of graphene/Al Composites.

Although experimental research is the main means of composite design, the study of composite materials by computational simulation has great economic and time advantages, especially for rare and precious metal composites. Song et al. [16] simulated the drawing process of nickel plated carbon nanotubes (CNTs) in Al substrate by molecular dynamics. By comparing the energy difference between the whole system before and after CNTs drawing, the influence of nickel layer on the interface binding force between CNTs and Al was studied. Xiao and Hou [17] studied the effect of carbon nanotubes on the tensile properties of Al based materials by molecular dynamics. It is found that the defect free carbon nanotubes can greatly enhance the failure stress and failure strain of Al based materials. Silvestre et al. [18] simulates the mechanical properties of carbon nanotube Al matrix composites during the compression process, and explains the role of carbon nanotubes in the enhancement process. Choi et al. [19] investigated the tensile property of CNT/Al composites based on molecular dynamics model, and found that the mechanical properties of the Al based materials can be effectively improved when the carbon nanotubes are increased to a certain amount. These results not only coincide with the experimental results, but also can help us better understand the changing mechanism of composites under loading, and provide theoretical support for the enhancement mechanism of nanofillers.

In this paper, the basic tensile properties and enhancement mechanism of GNP/Al composites materials are investigated based on molecular dynamics simulations. Through the analysis of the tensile process and microstructure evolution of composites, the important role played by the mechanical behavior of GNPs in composite materials is explored. This research can provide a theoretical basis for the design of stronger and tougher materials.

2. Model development

2.1. Simulation models

The molecular dynamics simulations soft of LAMMPS is adopted to investigate the enhancement mechanism of embedded GNPs on GNP/Al composite with different GNPs size and chirality, a series of molecular dynamics simulation are conducted under uniaxial tension loading. The simulation utilizes non-periodic and shrink-wrapped conditions. Four different models with varying GNPs geometry size are created in the simulations. A same Al matrix geometry is used with the dimension of 10.94 nm × 8.51 nm × 4.05 nm. A prism vacancy is created to accommodate the reinforced GNP, which is 1 Å larger than the GNP so as to allow the Al matrix can contain it, as shown in Fig. 1. The armchair GNPs of size 8.4 nm × 2.0 nm, 8.4 nm × 4.0 nm and 8.4 nm × 6.0 nm are placed in the vacancy. A zigzag GNPs of size 8.4 nm × 4.0 nm is also considered in the model to investigate the chirality effect on the enhancement of composites.

2.2. Potential functions

In the present study, an Embedded-Atom Method (EAM) potential is employed to define the interatomic interaction of Al atoms; a second-generation Reactive Empirical Bond Order (REBO) potential is utilized to define the C atomic interaction within the GNPs; a Lennard–Jones (LJ) potential is used to compute the force between Al-C atoms. Thus the system's total energy should be represented as:

$$E_{total} = E_{Al}^{EAM} + E_{C}^{REBO} + E_{Al\text{-}C}^{LJ} \tag{1}$$

The EAM potential can be formally written as a summation of pairwise interactions and embedding energy:

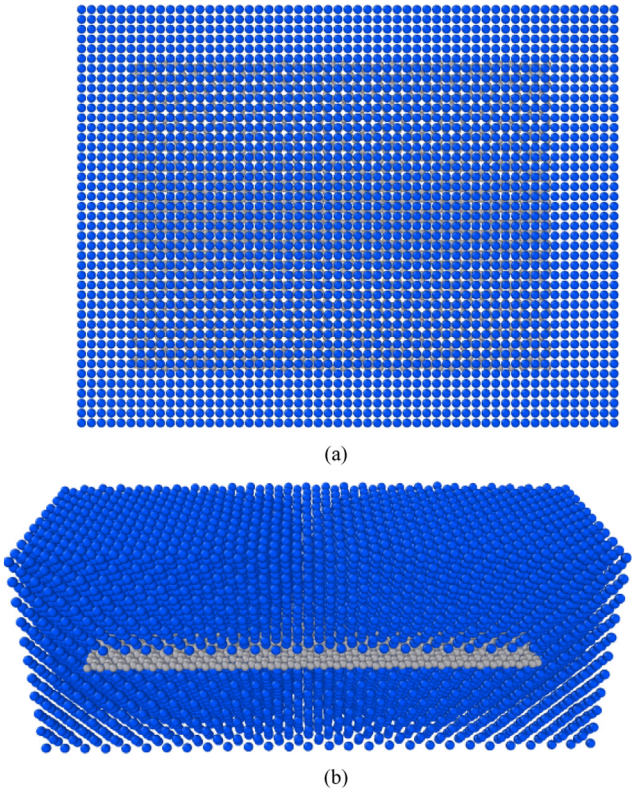

Fig. 1. The planform (a) and side elevation of center section (b) of the composite model that GNP embedded Al matrix.

$$E^{EAM} = \sum_i \left[\frac{1}{2} \sum_{j \neq i} \Phi(r_{ij}) + F(\overline{\rho}_i) \right] \tag{2}$$

$$\overline{\rho}_i = \sum_{j \neq i} \rho(r_{ij}) \tag{3}$$

where Φ represents the pair potential, which relates to the separation of atoms, r_{ij}; F is the embedding energy related to the density $\overline{\rho}_i$ as given in Eq. (3); ρ represents the atomic density function [20].

The Reactive Empirical Bond Order (REBO) potential is a semi empirical many body potential studied by Brenner et al. [21] The second generation REBO Potential is its further improvement and development and has become one of the most accurate potential functions that describe the hydrocarbon system [22,23]. Its function reads:

$$E^{REBO} = \sum_i \sum_{j>i} [V_R(r_{ij}) - B_{ij}^* V_A(r_{ij})] \tag{4}$$

where the r_{ij} represents distance between atoms i and j. The B_{ij}^* represents the bond-order parameter. $V_R(r_{ij})$, $V_A(r_{ij})$ represent interatomic repulsions and attractions, respectively [24].

The interactions between Al-C atoms are modeled with a 12-6 LJ potential. The function model is reads:

$$E^{LJ} = 4\varepsilon \left[\left(\frac{r_{ij}}{\sigma} \right)^{-12} - \left(\frac{r_{ij}}{\sigma} \right)^{-6} \right] \tag{5}$$

where the parameter ε and σ are energy scale parameters and collision diameter parameters, respectively [25]. For the interactions between Al-C atoms, $\sigma = 3.1325$ Å and $\varepsilon = 0.003457$ eV are adopted based on the earlier studied of Ashish et al. [26].

2.3. Simulation process

After the initial configuration is built, the initial model is fully relaxed under the set temperature and ensemble, so as to eliminate the