Molecular Dynamics Simulation of Mechanical Properties of Graphene/Magnesium Matrix Composites

Dunwei Peng [1,2], Qingwei Guo[1], Xiaopan Wang[1], Hua Hou[1,3], Yuhong Zhao[1,4,5*]
1 School of Materials Science and Engineering, Collaborative Innovation Center of Ministry of Education and Shanxi Province for High-performance Al/Mg Alloy Materials, North University of China, Taiyuan, 030051, China
2 School of Materials Science and Engineering, Xi'an University of Technology, Xi'an, Shaanxi 710048, China
3 School of Materials Science and Engineering, Taiyuan University of Science and Technology, Taiyuan, 030024, China
4 Beijing Advanced Innovation Center for Materials Genome Engineering, University of Science and Technology Beijing, Beijing, 100083, China
5 Institute of Materials Intelligent Technology, Liaoning Academy of Materials, Shenyang, 110004, China
*Corresponding address: e-mail: zhaoyuhong@nuc.edu.cn

Abstract: In this work, molecular dynamics simulations were used to investigate the effects of monolayer graphene (GR) with varying orientation angles on Mg-9Al-1Zn (AZ91 wt.%) on mechanical properties of magnesium alloy. The simulation results show that Young's modulus and tensile strength of AZ91/GR composites decrease gradually with the increase of the orientation angle of the 1LG. The Young's modulus and tensile strength of AZ91/GR composites can be improved by the 1LG orientation angle of 0°~10°, where the two are enhanced by 21.7% and 19. 7% respectively, at an orientation angle of 0°. However, the Young's modulus and tensile strength of 1LG are decreased for orientation angles of 20°~90°. It can provide some technical guidance for the experimental process design of AZ91/GR composites.

Keywords: AZ91 Magnesium matrix composites, Graphene, Molecular Dynamics, Mechanical property

1 Introduction

The research and development of graphene magnesium matrix composites can provide new solutions for the application of lightweight materials. In recent years, researcher found that the GNPs were aligned along the tensile direction, enhancing the strength of the graphene/magnesium matrix composites [1, 2]. However, the contribution of GNPs perpendicular to the tensile direction was minimal, limiting their ability to enhance the overall mechanical properties. The impact of graphene nanosheets at different angles to the stretching direction was not specifically addressed with current experimental equipment in detail. This paper focuses on modeling AZ91/GR composites with graphene nanosheets of varying orientation angles using molecular dynamics simulations to understand the tensile deformation mechanism.

2 Experimental procedure

This work is carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [3]. Ten groups of tensile models of AZ91/GR magnesium alloy composites with different orientation angles (θ = 0°, 10°, 20°, 30°, 40°, 50°, 60°, 70°, 80°, 90°) were designed in this study. The Mixed Element Atomistic Method (MEAM) [4] potential function is used in MD simulations to describe the interatomic interactions in Mg-Al-Zn alloys. At the same time, the interatomic interaction of GR is described by the Adaptive Intermolecular Reaction Empirical Bond Order (AIREBO) potential function [5]. In addition, the interactions between Mg-Al-Zn alloys and GR were described using the Lennard Jones (L-J) potential function [6] with the cutoff radius set to 1 nm. The specific energy and distance constants are as follows:
$\varepsilon_{Mg\text{-}C} = 0.0027$eV,$\sigma_{Mg\text{-}C} = 3.5015$ Å; $\varepsilon_{Al\text{-}C} = 0.035078$eV, $\sigma_{Al\text{-}C} = 3.0135$; $\varepsilon_{Zn\text{-}C} = 0.00265699$eV, $\sigma_{Zn\text{-}C} = 3.9735$ Å.

3 Result and discussion

Fig.1(a) shows stress-strain curves for AZ91/GR composites and AZ91 magnesium alloy with graphene monolayers with different orientation angles. The results show that the tensile strength of GR increases to 4.66 GPa at orientation angles of 0°and 10°, while it decreases when the angles range from 20° to 90°. In all models, the stress initially increases linearly with strain, following Hooke's law. The slope of the stress-strain curve during the initial elastic stage represents Young's modulus of the AZ91/GR composites. The results presented in Fig.1(b) indicate that Young's modulus of AZ91/GR magnesium composites is higher and the likelihood of deformation is reduced when the orientation angle of GR is at 0°,10°and 20°. Conversely, as the orientation angle is 30°~90°, Young's modulus decreases, leading to an increased likelihood of deformation. The Young's modulus of AZ91/GR magnesium alloy composites decreases as the orientation angle increases and tends to increase after surpassing 60°, but remains lower than Young's modulus of the AZ91 magnesium alloy. The results presented in Fig. 1(c) demonstrate that incorporating GR can improve the tensile strength of AZ91 magnesium alloy to 4.66 GPa. Furthermore, it is observed that as the orientation angle increases, there is a gradual decrease in the tensile strength.

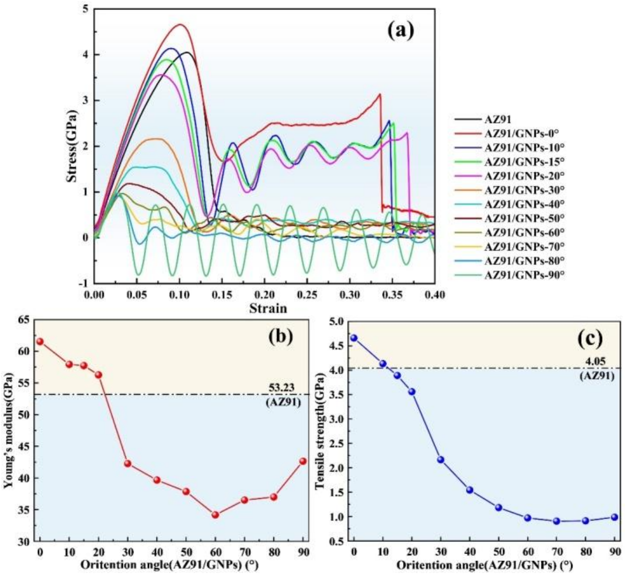

Fig.1 (a) The stress-strain curves of AZ91 alloy and AZ91/GR composites were measured at different orientation angles of GR; (b) The Young's modulus of the composite material depicted in the fig. (a); (c) The tensile strength of the composite material depicted in the fig. (a)

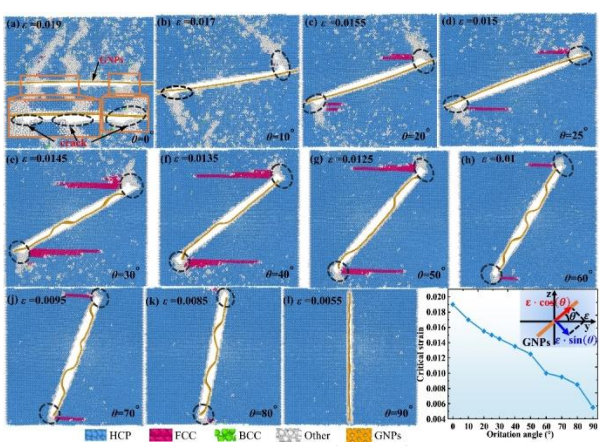

Fig.2 The evolution morphology of AZ91/GR composites with different orientation angles of GR under critical strain.

The evolution of morphology in AZ91/GR composites with varying orientation angles of GR under critical strain is depicted in Fig.2. The critical strain of AZ91/GR composites shows a distinct correlation with the orientation angle of GR. Specifically, a larger orientation angle of GR results in lower stress at the ends of the GR and a reduced critical strain. A simplified model is employed to elucidate the impact of orientation angle on the behavior of GNPs. The forces acting on the GR are resolved into components of $\varepsilon \cdot sin\,(\theta)$ and $\varepsilon \cdot \cos\,(\theta)$, where $0^{\circ} \ll \theta < 30^{\circ}$, causing the GR to extend along the $\cos\,(\theta)$ direction. As $30^{\circ} < \theta \ll 90^{\circ}$, $sin\,(\theta)$ becomes dominant, leading to the formation of local wrinkles in the graphene structure. This results in the bending and debonding of the GR in AZ91/GR composites. The simulation reveals that the critical orientation angle for GR is 30°. Furthermore, the critical strain of the AZ91/GR composite matrix decreases as the orientation angle of the GR increases, consequently reducing the load-bearing capacity of the GR.

4 Conclusion

(1)The strength of AZ91/GR-0° and AZ91/GR-10° single crystal composites surpass that of the AZ91 matrix magnesium alloy. As the orientation angle of GR increases (30°~90°), debonding occurs, leading to reduced tensile strength and increased susceptibility to deformation in AZ91/GR composites.

(2)The fracture time of AZ91/GR single crystal composites advances with higher orientation angles of GR. The impact of GR on the strength of AZ91/GR single crystal composites is primarily determined by the orientation angle of GR.

5 Acknowledgments

This work was supported by the National Natural Science Foundation of China (Nos. 52275390, 52375394), Key Research and Development Program of Shanxi Province (202102050201011, 2022ZDYF035).

References

[1] Rashad M, Pan F S, Hu H H, et al. Enhanced tensile properties of magnesium composites reinforced with graphene nanoplatelets[J]. Materials Science & Engineering A, 2015, 630: 36-44.

[2] Yuan Q H, Zeng X S, Wu J B, et al. Preparation and mechanical properties of graphene nanosheets reinforced AZ91 alloy composites[J]. Special Casting Nonferrous Alloys, 2016, 36: 282-286.

[3] Plimpton S, Fast parallel algorithms for short-range molecular dynamics[J]. Journal of Computational Physics. 1995, 117: 1-19.

[4] Dickel D E, Baskes M I, Aslam I, et al. New interatomic potential for Mg–Al–Zn alloys with specific application to dilute Mg-based alloys[J]. Modelling and Simulation in Materials Science and Engineering, 2018, 26: 045010.

[5] Stuart S J, Tutein A B, Harrison J A, A reactive potential for hydrocarbons with intermolecular interactions[J]. Journal of Chemical Physics, 2000, 112: 6472-6486.

[6] Zhou X, Liu X X, Mechanical Properties and Strengthening Mechanism of Graphene Nanoplatelets Reinforced Magnesium Matrix Composites[J]. Acta Metallurgica Sinica, 2020, 56: 240-248.