# Synergistic Crack Inhibition in 2024 Al-GNPs/TC4 Laminated Composites: Experimental, Phase-Field Modeling, and Molecular Dynamics Investigation

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**Abstract:** The Al layer always cracks first in Al/Ti LMCs due to its low strength. In this study, 2024 Al-GNPs/TC4 LMCs were prepared by replacing the conventional Al alloy with 2024 Al-GNPs composites. Its ultimate tensile strength of 757 MPa surpasses that of almost all other Al/Ti LMCs. The lamellar structure and GNPs were found to have a synergistic effect in enhancing the mechanical properties by inhibiting crack extension across and within the layers, respectively. The hindrance of crack extension by the lamellar structure is primarily due to strain delocalization in TC4, as confirmed by phase-field-crystal simulation. On the other hand, GNPs impede crack extension through passivation and deflection, which was revealed by molecular dynamics to be attributed to dislocation hindrance and load transfer.

**Keywords:** Laminated composites, Graphene, Phase-field simulation, Mechanical properties.

## 1 Introduction

Although the lamellar structure provides a significant strengthening effect, the performance limit of Al/Ti LMCs is constrained by the lower strength of the Al layer. Under stress, cracks tend to initiate in the Al layer first, which results in stress concentration in the Ti layer and ultimately leads to fracture failure of the Al/Ti LMCs.Compared with Al, aluminum matrix composites (AMCs) exhibit superior strength. It is thus speculated that replacing Al with AMCs may be an effective way to further enhance the performance of LMCs. Numerous studies have confirmed the feasibility of replacing Al with AMCs to enhance the strength of LMCs. However, the incorporation of granular reinforcing materials makes AMCs suffer from disadvantages such as transient damage, limited ductility, and poor processability. As a new type of reinforcing material, graphene nanoplatelets (GNPs) with excellent mechanical properties and unique lamellar structure are expected to improve the strength and ductility simultaneously [1]. This work reported 2024 Al-GNPs/TC4 LMCs with an ultimate tensile strength (UTS) surpassing that of almost all other Al/Ti LMCs. The correlation between the mechanical properties, microstructure, and crack extension of 2024 Al-GNPs/TC4 LMCs was investigated. The reason for the different crack evolution in Ti and Al was explained by the phase-field-crystal (PFC) method. The molecular dynamics (MD) method was used to analyze the mechanism of crack blocking by GNPs. In addition, the interfacial atomic diffusion behavior was investigated by the phase-field method. This work finds that GNPs and lamellar structure synergistically block the crack extension to break the performance limit of Al/Ti LMCs and provides a new idea for the design of LMCs.

## 2 Experimental procedure

The TC4 and 2024 Al-GNPs composites foils were surface-treated and stacked as shown in Fig. 1. After sintering in SPS, the 2024 Al-GNPs/TC4 LMCs were obtained.


**Fig. 1 Schematic illustration of the preparation process for 2024 Al-GNPs/TC4 LMCs.**

## 3 Result and discussion

The morphology of the 2024 Al-GNPs/TC4 LMCs is shown in Fig. 2a. The grains of the 2024 Al-GNPs composites are significantly larger than those of TC4, while the $Al_3Ti$ layer has the smallest grains. This formed a special structure with alternating coarse-fine grain distribution.

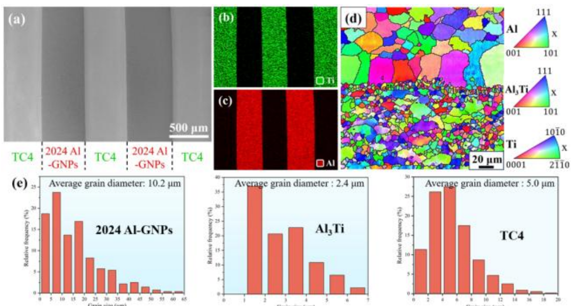

**Fig. 2 (a) SEM image of 2024 Al-GNPs/TC4 LMCs, EDS mapping of (b) Ti, (c) Al, (d) IPF map of the 2024 Al-GNPs/TC4 LMCs interface, (e) Grain size statistics of 2024-GNPs composites layer, Al3Ti layer, and TC4 layer.**

Figs. 3a$_1$-c$_1$ show the crack evolution without dislocation by phase-field simulation [2, 3]. The main crack propagates along the direction of the maximum shear stress and ultimately penetrates the whole layer. As the dislocation density increases, the dislocations act as sources of cracks and sprout microcracks, as shown in Figs. 3a$_2$-c$_2$. Microcracks disperse strain to prevent excessive crack extension caused by strain concentration, as shown in Fig. 3b$_2$ and its inset. This finding reveals that TC4 disperses local stress concentrations through uniformly distributed dislocations, thus avoiding the continuous extension of individual cracks.

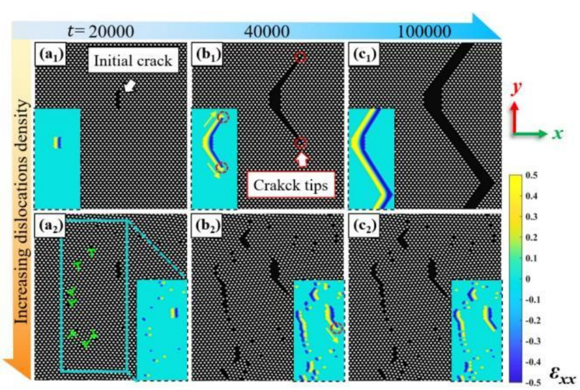

**Fig. 3 Crack evolution by Phase-field-crystal method. (a$_1$-c$_1$) Crack evolution without dislocation, (a$_2$-c$_2$) Crack evolution with high-density dislocations, Insets show the strain field distribution: blue and yellow represent compressive strain and tensile strain, respectively.**

A high-density dislocation region was observed near the GNPs, which contains a large number of dislocations and dislocation tangles. This is attributed to the obstruction of dislocations by GNPs. Molecular dynamics confirms that GNPs hinder the connection between dislocations and crack tips.

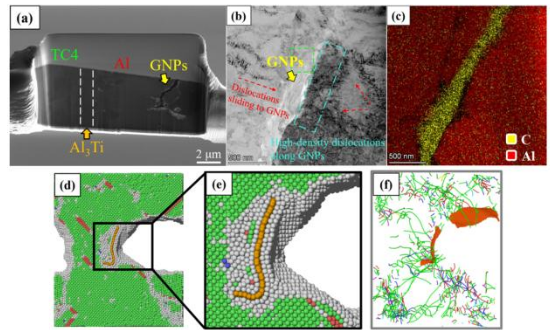

**Fig. 4 (a) FIB sample of 2024 Al-GNPs/TC4 LMCs, (b) Dislocation distribution around GNPs, (c) distribution of Al and C elements, and (d)-(f) Molecular dynamics study of GNPs hindering dislocation motion**

## 4 Conclusion

(1) Dense microcracks are generated in the TC4 layers to compensate for the strain difference.
(2) GNPs were found to prevent crack extension within the 2024 Al layer by passivating and deflecting.
(3) Stress is transferred from the matrix to GNPs, which disperses the stress concentration.
(4) GNP prevents dislocations from connecting with the crack tip.

## 5 Acknowledgments

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