Multi-scale strengthening and toughening mechanism for graphene derived layer-by-layer materials

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Abstract

Graphene derived layer-by-layer materials (papers, films, fibers, etc.) have attracted many research interests for their broad application prospects in flexible electronics, biomedicine, energy storage devices and so on. These materials usually feature layer-by-layer (LBL) microstructures with single sheet spanning over hundreds of micrometers. However, compared with monolayer graphene sheet, the mechanical properties of these materials reduce more than one order of magnitude due to the weak interlayer interactions between the graphene sheets. Thus, scientists have tried different experimental methods to improve the overall mechanical behaviors of graphene derived materials, such as interlayer crosslinking, microstructure adjusting, defect controlling. However, a multiscale toughening and strengthening strategy for graphene derived LBL materials is still in lack.

In this study, a multi-scale theoretical model was proposed to describe the load transfer from graphene sheet to macroscopic materials, as well as to provide practical advice to optimize the manufacturing processes for elevated mechanical properties. Firstly, a nonlinear spring-bead model was proposed to capture the deformation and failure modes on the molecular scale. Combining the spring-bead model with the concepts of self-healable interlayer crosslinks that mimicking hydrogen bond or ionic bond, we have distinguished three microscopic failure modes for graphene derived LBL materials, including intralayer fracture of graphene sheets, interlayer sliding with and without reconstruction. The results show that with the introduction of the self-healable crosslinks, the toughness of graphene LBL materials significantly improves (i.e. theoretical limit of plastic strain 50%) compared with those without self-healable crosslinks. Further, the nonlinear spring-bead chains with different dimensions were combined to describe the mechanical properties of the microstructures. Finally, we presented a microstructural optimization design method to obtain the optimal macroscopic strength and toughness for graphene-polymer composites with different volume fractions of graphene.

This study provides a multi-scale method to describe the processing-microstructure-performance relationship for graphene derived LBL materials. The results obtained may shed useful insights into the processing and optimization of graphene derived LBL materials.

Keywords: Graphene derived materials, Multi-scale model, mechanical properties, optimization.