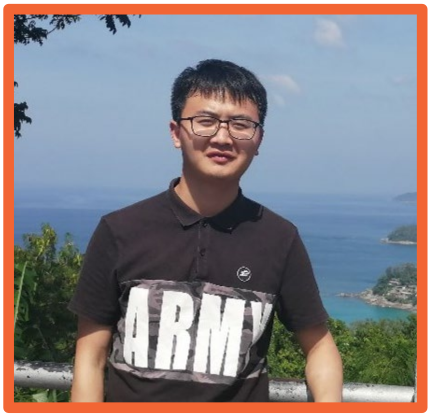
Graduate Student Research Seminar

Spring 2022

Investigation of Dynamic Impact Response of PMMA-Graphene Layered Nanocomposites Using Molecular Dynamics Simulations

Zhangke Yang (PhD student)

Advisor: Dr. Zhaoxu Meng



Monday, April 11th

3:00 pm (EST) – 132 Fluor Daniel Building

Abstract

Nanostructured polymer composites show superior energy dissipation capability with the advancement of the micro-projectile impact testing method. However, the detailed stress wave propagation and dynamics failure mechanisms during the extreme rate impact loading process have remained elusive. I will report our recent effort in understanding these mechanisms through the lens of molecular dynamics (MD) simulations. Specifically, we have constructed representative layered nanocomposites consisting of PMMA and graphene by using their corresponding coarse-grained models and applied MD simulations to study their dynamic impact response. The nanocomposites are built by embedding parallel and evenly spaced graphene layers into the PMMA matrix. Simple Lennard-Jones potential is employed to describe the interfacial interaction between PMMA and graphene. Shock waves are initiated in the thickness direction with a rigid piston moving at a high velocity and then released after a certain period. The other two directions are set to be periodic and infinite. By analyzing the spatiotemporal distribution of tensile stress and cross-section density, we find that the embedding of graphene layers can significantly affect the spallation of the nanocomposites by altering the strength of the reflected and released stress waves. The underlying mechanism is that the internal interfaces between graphene and PMMA partially reflect and thus attenuate the stress waves. Our results also indicate that the wave reflections by the graphene layers can increase the overall propagation distances of the original stress waves and consequently increase the dissipated energy. Furthermore, we find that the interfacial energy between PMMA and graphene plays an important role in the energy dissipation process, especially with densely distributed graphene layers. Our study provides insights into the development of nanocomposites with excellent impact resistance and energy dissipation by controlling the configuration and distribution of the rigid nanofillers in a soft matrix and their interfacial interactions.

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