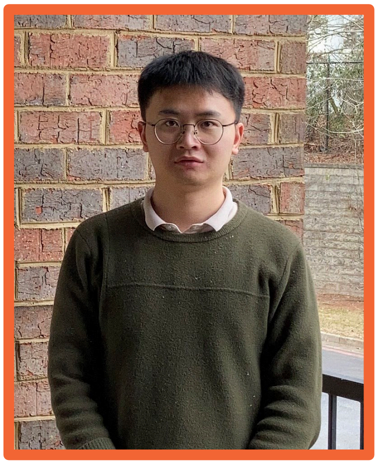
Graduate Student Research Seminar

Spring 2023

Designing Method Based on Shock Theory and Coarse-grained Molecular Dynamics for Layered Nanocomposite Films



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Monday, February 27th

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

Abstract

Layered nanocomposite films are inspired from nacre, a natural material that shows superior toughness and strength under dynamic loading. Our previous computational research on this type of nanocomposite films has shown that the interfaces between the layers have significant influences on the propagation of the shock wave generated by impact. The wave reflections occurred at layer interfaces change the overall propagation path as well as wave strength spatiotemporally. This can lead to multiple sub-waves and the potential interactions between them, such as the superposition of two sub-waves. The wave reflection mechanism in layered nanocomposite films and the resultant forms of sub-waves make the wave propagation process rather complex than that in films made up of homogeneous materials. Thus, the layered nanocomposite film's mechanical response under dynamic loading is totally different from homogeneous films and has been shown to be largely dictated by its nanostructure, while being certainly related to the properties of its constituent materials. This feature of the layered nanocomposite film provides us with means to control its mechanical response through tuning its nanostructure. However, a guidance on how to conduct such a tuning or designing process is still not clear to us. In this work, we try to approach this end by using continuum shock theory in association with coarse-grained molecular dynamics. First, we review the one-dimensional shock theory in a thorough way. Then, we discuss the applicability of this theory to the description of wave propagation process in layered nanocomposite films. Finally, we compare the two methods regrading their strength and drawbacks, respectively, and explore where we need to combine them and how to do that.

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