Mechanical Engineering Doctoral Defense

Multiresolution Coarse–grained Modeling of the Microstructure and Mechanical Properties of Polyurea Elastomer

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Abstract

Polyurea is a highly versatile material used in coatings and armor systems to protect against extreme conditions such as ballistic impact, cavitation erosion, and blast loading. However, the relationships between microstructurally-dependent deformation mechanisms and the mechanical properties of polyurea are not yet fully understood, especially under extreme conditions. In this work, we develop multi–scale coarse–grained models to probe molecular dynamics across the wide range of time and length scales that these fundamental deformation mechanisms operate. In the first of these models, we develop a high–resolution coarse–grained model of polyurea, where similar to united–atom models, hydrogen atoms are modeled implicitly. This model was trained using a modified iterative Boltzmann inversion method that dramatically reduces the number of iterations required. Using this model, we demonstrate that multiblock systems evolve to form a more interconnected hard phase, compared to the more interrupted hard phase composed of distinct ribbon–shaped domains found in diblock systems. Next, a reactive coarse–grained model is developed to simulate the influence of the difference in time scales for step–growth polymerization and phase segregation in polyurea. Analysis of the simulated cured polyurea systems reveals that more rapid reaction rates produce a smaller diameter ligaments in the gyroidal hard phase as well as increased covalent bonding connecting the hard domain ligaments as evidenced by a larger fraction of bridging segments and larger mean radius of gyration of the copolymer chains. The effect that these processing–induced structural variations have on the mechanical properties of the polymer was tested by simulating uniaxial compression, which revealed that the higher degree of hard domain connectivity leads to a 20% increase in the flow stress. We conclude with a hierarchical multiresolution framework to fully link coarse-grained molecular simulations across a broader range of time scales, in which a family of coarse– grained models are developed. The models are connected using an incremental reverse–mapping scheme allowing for long time scale dynamics simulated at a highly coarsened resolution to be passed all the way to an atomistic representation.

October 15, 2020; 1 PM;

Zoom Link: https://asu.zoom.us/j/4837130047