BRIDGING BETWEEN MOLECULAR TO COMPONENT SCALES IN MULTISCALE MATERIAL MODELING

Victor Oancea, Tod Dalrymple, Huidi Ji, Jing Bi, Sakya Tripathy

Dassault Systemes, SIMULIA

James Wescott, Stephen Todd

Dassault Systemes, BIOVIA

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ABSTRACT

Since the invention of optical magnification and later the microscope, researchers have been observing the microstructure of matter and materials. Robert Hooke, of Hooke's Law fame, published his book *Micrographia* in 1665, in which he described the cellular microstructure of cork. The field of metallography as the study of the physical structure of metals was already established in the nineteenth century. Just as the computer and finite element analysis modeling have allowed us to mathematically model and simulate a structure at the continuum scale, so to the advent of atomistic, or molecular computer modeling and simulation have allowed us to peer into the microstructure, or nanostructure of materials. Most materials have some complexity of structure at the nano or micro scale that influences their behavior at the continuum level. To enable continuum models to be built that capture this complexity it is necessary to bridge the gap between molecular scale models and the continuum. This approach is likely to be particularly helpful for simulations of composite materials and materials involved in additive manufacturing processes. Classical and mesoscale simulations based on molecular structure can be used to predict key properties, including cohesion and wetting, mechanical behavior, diffusion, adhesion at surfaces and phase separation. Such simulations can be leveraged in finite element (FE) simulations through homogenization of the predicted material structure and through use of the simulated material properties for FE input. In this paper, we will work through and extend one particular multi-scale workflow starting with the construction and characterization of a thermoplastic co-polymer at the atomistic level and ending with a macroscopic part level simulation using finite element modeling. We will apply molecular dynamics to understand the nanostructure and mechanical properties of the constituents of polyurea, a microphase-segregated polymer. This nanoscale information will then be used at the FEA level to construct continuum level material models for the polyurea material.