Thermophysical Property Prediction of Aerospace Thermoplastic Polymers with Coarse-grained Models

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Thermoplastic polymers are gaining traction as replacements for thermosets as the matrix phase in aerospace composite materials due to their superior mechanical properties, recyclability, and improved joining through fusion welding. In parts manufactured from fusion welding, entanglements across the interface determine mechanical strength. It is therefore important to understand how entanglements develop during fusion welding at the molecular level. Molecular dynamics simulations give insight into the fusion welding process, but can be limited by the long time scales required for modeling polymer diffusion and entanglement. Additionally, accurately and reproducibly modeling a complex process such as fusion welding of polymers creates unique implementation and software design challenges.

In this work, we develop a transparent and reproducible software package with functionality to initialize and equilibrate both atomistic and coarse-grained polymer systems that feed into a fusion-welding and mechanical testing workflow. We address the time and length scale challenges using multi-state iterative Boltzmann inversion (MSIBI) to create a coarse-grain models of commonly used aerospace thermoplastics poly(etherketoneketone) (PEKK) and poly(phenylenesulfide) (PPS). We validate the coarse models against experimental measurements including glass transition temperature, density, and melting behavior. We conclude with a discussion of the performance benefits and workflow limitations.