Advancing Molecular Dynamics Simulation and Experimentation to Expedite Development of Next-Generation Aerospace Composite Polymer Matrices

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ABSTRACT

Molecular dynamics (MD) simulation is seeing new levels of use by scientists and engineers to rapidly advance multi-scale development platforms for Horizon-III aerospace materials. MD simulation provides new pathways to expedite development while reducing experimentation and cost for preparing high-performance glassy polymer networks employed as polymer matrices and precursor polymers employed within advanced composite structures. These polymers and precursors are notoriously difficult and costly to develop since the ultimate vitrified amorphous solids are insoluble making them difficult to analyze and reproduce. Peculiarities connected with the extent of conversion, kinetics, cure-path dependencies, phase separation, fillers and toughenners collectively create a particularly challenging area of polymer science and engineering. Collaborations with global leading defense and aerospace groups has validated MD simulation methods to pre-screen molecular designs, simulate thermal and mechanical properties, and visualize equilibrated and non-equilibrated architectures to guide and inspire synthetic efforts prior to conducting physical experiments. We will review our observations, deliberate contemporary needs and discuss future directions to advance multi-scale modeling frameworks which link quantum/molecular level events with continuum level structural performance of next generation aerospace materials.