Utilization of Molecular Simulations in Aerospace Materials: Molecular Dynamics Simulations of Thermoset Resins

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Molecular simulations have proven to be useful in improving the understanding of aerospace materials, particularly thermoset resins. Simulations tools such as molecular dynamics have allowed for the exploration of the relationship between monomer structure and bulk properties; relationships which in turn are useful in new resin development. In order to be able to simulate thermoset resins, a resin construction method that allows for a wide variety of monomers to be modeled and results in good property (e.g., density) agreement with experiments was developed. Simulation methods were also developed for resin equilibration and bulk property estimation, including Tg and stress/strain behavior. This poster will describe the construction and simulation method used for thermoset resin modeling, as well as other uses of molecular simulations such as exploration of graphite/resin interactions. This recent work in material simulations demonstrates that the future of aerospace materials development includes simulation tools.