Classical All-Atom Models for HTPB-Based Binders and Ammonium Perchlorate

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Solid propellants are essential to the Air Force because of their low risk, high performance, competitive cost, storability, and near-instant readiness. Solid energetic compounds are generally brittle, so to reduce the brittleness of the propellant a polymer is incorporated to form a composite propellant. Commonly used composite propellants contain ammonium perchlorate (AP) suspended in a polymeric binder, such as hydroxy-terminated polybutadiene (HTPB)-based polyurethanes cured by a diisocyanate such as isophorone diisocyanate (IPDI). The unsaturated nature of the polybutadiene repeat unit makes HTPB susceptible to thermo-oxidative degradation, and therefore loss of mechanical properties and subsequent failure of the propellant. It is desirable to artificially control the type and quantity of degradation products and see how the resulting mechanical properties of the polymeric binder are affected by utilizing molecular simulation. Interfacial phenomena involving the polymeric binder and AP, such as debonding, are also of interest. Before introducing degradations to the polymeric binder, development of new molecular models and force field parameters is necessary to perform molecular simulations with fully atomistic detail. Our HTPB model demonstrates associative behavior for the hydroxyl groups in the HTPB melt. Using the OH spatial distribution as a template for cross-linking locations, IPDI is used to cure the HTPB into an elastomer. The binder is subsequently subjected to deformation simulations to compute mechanical properties at various temperatures. Future work is discussed for the parameterization of AP–HTPB interfacial interactions for studying debonding phenomena.