Simulations of polymeric materials at the U.S. Army Research Laboratory

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Polymers, polymer networks, and their composites are widely-used in a variety of military and industrial applications, yet many of these materials have not been designed to function in extreme mechanical or thermal environments. The design space of polymeric materials is tremendous, and large improvements in quasi-static and high strain-rate properties may be possible through optimization of chemistry and processing. Molecular simulation techniques - such as density functional theory, classical molecular dynamics, and coarse-grain dynamics - are valuable both in guiding experiments through predictive screening of properties, and in rationalizing the behavior of materials already known to be 'high-performers'. In this presentation, results and limitations of atomistic- and meso-scale simulations are discussed, including mechanical and shock properties of several amorphous and semi-crystalline polymers, and thermosetting networks. The mechanical properties of glass-forming polymeric materials are shown to be particularly sensitive to accelerated strain rates and cooling rates, with a wide range of stress responses possible. Further, several unique challenges in generating molecular structures of polymers will be discussed along with possible solutions.