Molecular Simulation of Shock Hugoniot for Polymers T. SIRK, T. CHANTAWANSRI, E. BYRD, B. RICE, J. ANDZELM, Army Research Laboratory — The behavior of polymers under extreme conditions (high pressure and temperature) is of interest for a variety of applications, such as polymer-bonded explosives, coatings, adhesives, and light-weight armor. Material properties and response at extreme conditions can be determined through shock experiments, which are often difficult to measure experimentally because of difficulties in traversing a large range of pressures (up to hundreds of gigapascals) and temperatures (thousands of kelvin) with available instrumentation. In addition, interesting behavior, such as observed behind a shock front, occurs at extremely short time- and length-scales (nanoscale), which poses problems in characterizing the material using current experimental capabilities. To further understand shocked systems, simulation methods such as molecular dynamics (MD) and quantum mechanics (QM) can be used to provide insight into atomic-level phenomena. Using classical MD and QM, we have calculated the principle shock Hugoniot curves for four polymers: poly[methyl methacrylate], poly[ethylene], poly[styrene], and hydroxyl-terminated poly[butadiene]. In the MD calculations, we considered both a non-reactive (i.e. PCFF) and reactive (i.e. ReaxFF) forcefield, respectively, where calculations were performed in LAMMPS. The QM calculations were performed with density functional theory (DFT) using dispersion corrections as implemented in CP2K. We have applied both atom centered pseudopotentials (DCACPs) and Grimme van der Waals corrections in our study. Overall, results obtained by QM show much better agreement with available experimental data for the range of up to 20 GPa than classical force fields. At pressures where reactions can occur the short simulation time available in MD modeling prevents us from fully exploring possible reaction pathways.

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