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Establishing structure-property-performance linkages for energetic materials SIDHARTHA ROY, OISHIK SEN, NIRMAL RAI, MIN-YEONG MOON, KYUNG CHOI, University of Iowa, CHIRSTOPHER MOLEK, ERIC WELLE, ANGELA DIGGS, DAVID HARDIN, Air Force Research Laboratory, H S UDAYKUMAR, University of Iowa — This work details a framework for establishing structure-property-performance linkages for energetic materials using a multi-scale simulation approach. A MESo-informed Ignition and Growth model (MES-IG) is used to quantify performance, i.e. loading conditions for shock-to-detonation transition. Physical descriptors are used to characterize SEM-imaged microstructures for three classes of HMX based pressed energetics. Meso-scale reactive void collapse simulations are performed to establish the link between the meso-structure and meso-scale physical response; structure-property linkages. The structure-property linkage is then encapsulated in a surrogate model for the rate of ignition and growth of reaction fronts. The machine-learned surrogate models are used to provide closure at the macroscale, resulting in microstructure aware simulations of shock-to-detonation transition. James curves and pop plots are developed for each Class of the pressed HMX and compared with experimental data. The uncertainty due to stochastic micro-structures are quantified by constructing probability distributions of the microstructural descriptors and quantifying the effects of individual descriptors on the macroscale QoIs. This framework can be used to design a wide variety of energetic materials.

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