

---

# Microstructure-sensitive modelling of solid explosives under mechanical impulse

Dr. Ushasi Roy\*<sup>1</sup> and Navankur Shrotriya

<sup>1</sup>Department of Mechanical Engineering, Indian Institute of Technology Kanpur – India

## Abstract

Designing solid explosives for insensitive munitions is an essential exercise to reduce the wastage of human and material resources due to catastrophic accidents involving unexpected explosions. Some standard tests and protocol exist to test the insensitivity of the solid explosives towards sudden mechanical and thermal impulse. The novel materials must qualify tests, specifically, the bullet/fragment impact test for structural integrity. However, performing such tests with explosives is not only expensive, at times, almost impossible in terms of hazards and threats it offers. This shows the necessity of a predictive computational model that could replicate these insensitive munitions tests reliably and thereby reduce the number of experiments needed to qualify a novel material for insensitive munitions. The hydrocodes currently available to predict the detonation behavior of explosives do not take into account the microstructural details of the solid explosives and therefore cannot be appropriately used for novel materials' design purposes. To design next generation solid explosives as insensitive munitions, it is customary to establish the relation between microstructural features and the detonation behavior at the macro-scale. The macro-scale characteristics of solid explosives are largely influenced by the equations of states before and after chemical reaction initiates. These constitutive laws are still not known as a function of the composite's microstructure. Therefore, in this work, we develop a microstructure-sensitive Finite Element based model that predicts the constitutive laws at the macroscale as a function of the microstructure. A solid explosive is primarily made up of energetic particles embedded in polymer matrix. We use a simple HTPB-estane type polymer bonded explosive (PBX) for our study. However, the model is capable of accounting for any other phases that may be present in PBX like Ammonium Perchlorate and so on. Statistically similar microstructures are generated to account for stochasticity in performance of these composites. Different distributions of energetic grains are studied to delineate the influence of microstructures on the deformation behavior of these composites under high strain rate loading. These digitally generated microstructures are then subjected to high strain rate periodic boundary conditions to study their deformation behavior. Cohesive elements are employed to allow fracture during loading to happen at arbitrary locations. Different constitutive laws are defined for each of the constituents of the microstructure, as well as the cohesive surfaces. The overall stress-strain responses of the microstructures are recorded along with their local heterogeneous response. Master curves are drawn to obtain the equations of state at the macro-scale as a function of their microstructure. Temperature evolution is also studied during this high strain rate loading. Heating throughout this adiabatic loading is effected through inelastic dissipation and frictional dissipation at the cracked surfaces. This leads to generation of hotspots. The hotspot maps under different loading conditions are also extracted to facilitate identification

---

\*Speaker

of the initiation of chemical reaction in these composites. Our simulation stops before the chemical reaction initiates. This thermo-mechanical model helps in delineating the effects of microstructure on the macro-scale equations of state of the unreacted solid explosive and on the probability of ignition initiation. The model has the capability to aid in novel composites design for insensitive munitions.