20th European Mechanics of Materials Conference - EMMC20
Florence, Italy | May 27th-29th, 2026
www.emmc20.unifi.it

A computational framework for coupled thermo-mechanical-chemical response of energetic materials under low velocity impact

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Paper ID: 513
Symposium S10: Coupled problems in material mechanics

Abstract

Ignition initiation of energetic materials under accidental low velocity impact remains a critical safety concern particularly in the presence of microstructure defects such as preexisting crack void and particle morphology irregularities. Although detonation is commonly associated with high velocity loading, experimental evidence shows that localized hotspots formation under low velocity impact can potentially trigger unintended ignition, therefore multi physics multi scale micro sensitive models are necessary to assess probabilistic detonation behaviour under low velocity impact. This predictive model requires to be robust and computational efficient to further contribute towards accelerated development of insensitive mutations In this work, we focus on polymer bonded explosives (PBXs) particularly HMX slygard composite. We obtain hotspot maps under low velocity (50m/s - 200 m/s) impact through solving thermo-mechanical-chemical response of the system. The objective is to understand sub-critical ignition mechanisms arising under nominally benign mechanical loading, where localized fracture and heating process govern damage accumulation and hotspot ignition. The proposed computational framework integrates mechanical deformation, thermal evaluation and chemical reaction kinetics within a unified numerical formulation implemented in Abaqus/Explicit. Dynamic phase field fracture is introduced using a thermal analogy, in which the phase field fracture governing equations is reformulated as an equivalent heat balance type equation.

This strategy enables efficient implementation within commercial finite elements software like Abaqus without relying on dedicated Multiphysics solvers. Coupling between physical fields is achieved through parallel cloning of computational meshed. The VUMAT subroutine models the purely elastic constitutive behaviour of microstructural constituents (PBXs) while computing strain energy degradation as the phase-field fracture driving force. The phase field evaluation is solved using VUMATHT via the thermal analogy. Frictional heat generation is modelled through phenomenological contact-based formulation, this includes evolution of crack pressure and velocity jump across cracked surfaces and frictional heat generation therein are tracked. Also, chemical heat release governed by a single step Arrhenius reaction model is modelled using cloning Data exchange between subroutines occurs via shared SDVs and a common subroutine. The framework successfully captures how fracture, frictional heating and local chemical reactions all interact during low velocity impact dynamics. Our results show that pre existing cracks particle shapes and the binder explosive interfaces play a key role in hotspot formation this method offers an efficient computational alternative to cohesive zone models or fully reactive simulations when studying accidental ignition in energetic composites.

Keywords:

PBX Thermo-mechanical-chemical coupling Phase Field Fracture Finite Element method Multi Scale Energetic Materials