Macroscopic ignition thresholds – microstructure relations for energetic materials under shock loading

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Abstract

Energetic materials (EM) have a wide range of applications such as propellants, fuels, explosives, and energy source for automobile air bags and pyrotechnics. Technical challenges for the design of EM include optimization with minimal trade-off among (1) performance – how to increase the energy content of EM and the delivery of power; (2) reliability – how to accurately control intended ignition and avoid accidental ignition; and (3) how to ensure the survivability and integrity of EM against mechanical (e.g., impact, accidental loading) insults? Solutions to these challenges require the establishment of precise conditions for the ignition of EM.

The establishment of macroscopic engineering-level ignition thresholds for EM in terms of microstructural attributes is an important objective for materials science and engineering, because microstructure-performance relations are essential to the design of new materials. Many mathematical relations or criteria have been proposed to quantify the thresholds, with the relations developed by James [1] and Walker and Wasley [2] being the most commonly used. The James relation describes experimental data using two macroscopic state variables: power flux and energy fluence. Walker-Wasley type relations are expressed in terms of input stress and load duration. So far, determination of such thresholds has been exclusively an experimental endeavor which is expensive, time-consuming, and possible only for samples in actual existence.

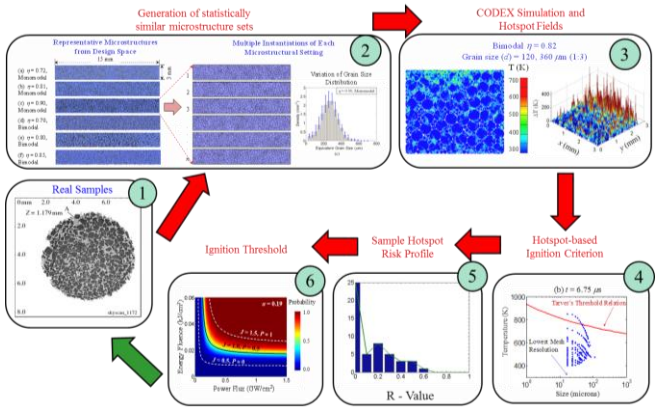

Fig 1. A computational approach for predicting the probabilistic ignition behavior of EM

Theoretical or computational prediction of the thresholds has hitherto been more a desire than reality. We have developed an approach to computationally establish these ignition thresholds as functions of material microstructure attributes and constituent properties (Fig. 1). The simulations explicitly account for not only microstructure and constituent properties, but also interfacial responses between the constituents. The framework captures processes responsible for the development of hotspots and damage. The specific mechanisms tracked include viscoelasticity, viscoplasticity, fracture, post-fracture contact, frictional heating, and heat conduction. The probabilistic analysis uses sets of statistically similar microstructure samples to directly mimic relevant experiments for quantification of statistical variations of material behavior due to inherent material heterogeneities. This capability has been used to predict the James and the Walker-Wasley ignition thresholds for pressed granular explosives based on HMX (octogen) crystals and several polymer-bonded explosives (PBXs) under a wide range of shock and non-shock loading. The ignition probability based on the James threshold is

$$\mathscr{P}(E,\Pi)=\frac{1}{2}+\frac{1}{2}\operatorname{erf}\left[\frac{1}{\sqrt{2}\sigma}\left(\frac{E\Pi}{\Pi E_c+E\Pi_c}-1\right)\right]. \tag{1}$$

The ignition probability based on theWalker-Wasley threshold is

$$\mathscr{P}(P,\tau)=\frac{1}{2}+\frac{1}{2}\operatorname{erf}\left[\frac{1}{\sqrt{2}\sigma}\left(\ln(P^2\tau)-\ln C\right)\right]. \tag{2}$$

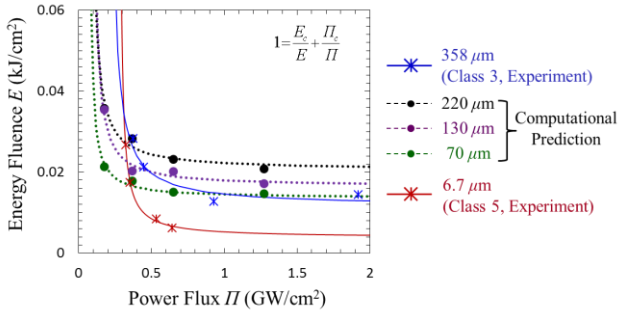

Fig 2. Computationally predicted 50% ignition thresholds from all grain sizes analyzed and experimentally measured thresholds for Class 3 and Class 5 HMX

The 50% ignition thresholds for three sets of pressed HMX samples with average grain sizes of $d_{avg}=70,130,\text{and }220\,\mu\text{m}$ are shown in Fig. 2 [3]. In general, a higher loading rate (power flux) results in a lower energy required for ignition (lower energy fluence). For a given loading rate (power flux), smaller grain sizes lead to lower ignition thresholds. The predicted initiation threshold obtained from the calculations are compared to the results from experiments. The trends observed in the computational predictions are in good agreement with those observed in experiments, as shown in Fig. 2. Moreover, the computationally predicted thresholds for the different grain sizes lie in the same range as the thresholds obtained by experiments for HMX

with grain sizes of $d_{avg} = 360\,\mu\text{m}$ and $d_{avg} = 6.7\,\mu\text{m}$. The predicted initiation thresholds for PBX 9404 and ignition probabilities are also in good agreement with results from shock experiments reported in the literature (Figs. 3-4). The framework also lends itself to the analysis of effects of microstructure defects in the forms of transgranular cracks and interfacial debonding sites. It has been found that higher defect levels correspond to higher impact sensitivity, implying that materials with more initial defects have lower ignition thresholds. This trend is more pronounced at lower load intensities. At higher load intensities, the effects of initial defects diminish as the effects of intrinsic heterogeneities in the microstructure dominate.

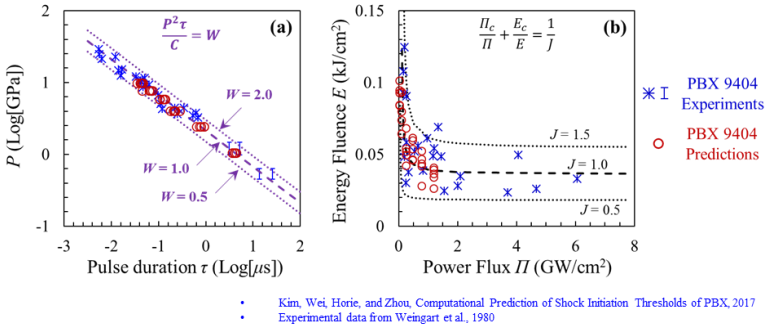

Fig 3. (a) Modified Walker-Wasley relation and (b) modified James relation

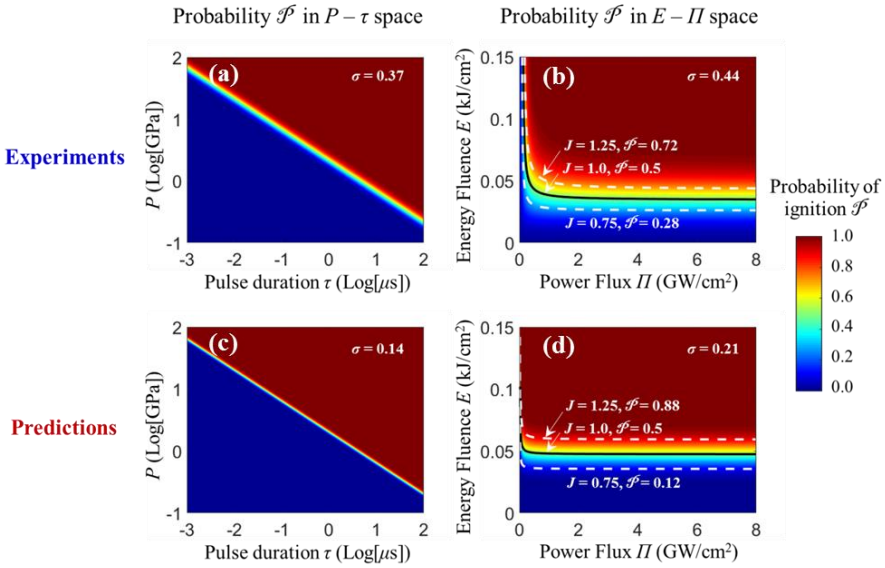

Fig 4. Ignition probability distribution maps, (a-b) as obtained from experiments in the (a) pressure – pulse duration ($P - \tau$) space and (b) energy fluence – power flux ($E - \Pi$) space, and (c-d) as predicted from simulations in the (c) pressure – pulse duration ($P - \tau$) space and (d) energy fluence – power flux ($E - \Pi$) space.

Calculations show that material microstructure attributes significantly affect the macroscopic ignition behavior of energetic materials. The capability to computationally predict the macroscopic engineering material response relations out of material microstructures and basic constituent and interfacial properties lends itself to the design of new materials as well as the analysis of existing materials.

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References

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