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A model for hot spot formation in shocked energetic materials

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ABSTRACT

Shock initiation and detonation are often attributed to wave interactions in the micro-structure of condensed materials, which involve complex thermo-chemical, fluid and structural processes. Due to their broad range of scales, the simulation of hot spot formation, reaction growth, and transition to detonation is therefore rendered challenging. The extension of these complex couplings to simulate full-scale tests is prohibitively costly. This paper introduces a hot spot formation model to account for heterogeneous effects based on physical and chemical properties. The formulation is first evaluated in a HMX (cyclotetramethylene-tetranitramine) sample where hot spots are known to form due to void collapses. Transition to detonation is achieved with impact pressures that match those found in experiments. Parametric studies are performed to determine the effects of the void size and population on the sensitivity of the material. Then, the same hot spot model is used to study detonation in nanocrystalline PETN (pentaerythritol-tetranitrate) where heating is primarily the result of grain boundary effects such as friction, plasticity, and deformation. The inclusion of the hot spot model increases the sensitivity of the material and predicts shock pressures, again similar to experimental values. Finally, a sensitivity analysis of the results is performed to assess the uncertainty in the input variables of the model and to identify the critical parameters with implications on the accuracy of the results.

1. Introduction

The emergence of new high explosive materials calls for the development of improved numerical techniques to predict their performance and sensitivity. Recent years have seen a drive towards the development of insensitive munitions, which are energetic materials with a reduced sensitivity to accidental stimulation. With applications in propulsive devices, mining, and development of weapon systems, understanding the mechanisms that influence sensitivity has become a topic of interest within energetic materials research. This study presents a numerical approach to predict the sensitivity and performance of energetic materials with emphasis on hot spot formation processes.

In energetic materials, particularly those with crystalline structures, shock sensitivity is greatly influenced by localized temperature spikes known as hot spots. First suggested by Bowden and Yoffe [1,2], hot spot formations are believed to dramatically increase the sensitivity through localized ignition of the material, which otherwise has a bulk temperature that is rather too low to ignite. These formations are a result of shock wave interactions with defects or voids at the scale of individual particles, referred to as the micro-scale. Also observed in the Deflagration-to-Detonation Transition (DDT) in premixed gaseous mixtures, hot spots are responsible for the onset of the development of the detonation front [3]. Here, their formation is due to the interactions of the flame generated shock waves with obstacles and sharp edges. Figure 1 presents a schematic diagram of the Shock-to-Detonation Transition (SDT) process due to the formation of hot spots [1,2,4]. The mechanisms involved in these formations undergo various mechanical, thermodynamic, and chemical processes such as visco-plastic heating, phase change, shear heating, condensed phase decomposition, gas phase compression, and inter-particle impact [5–8]. These phenomena occur due to the heterogeneous nature of the energetic materials and are still not very well understood.

Many experimental studies show a clear correlation between internal defects and sensitivity [9,10]. These investigations examine the effects of internal defects as well as inter-granular voids with varying population, size and even shapes [11]. Among the well known findings is that void size has a strong influence on sensitivity, where larger defects require lower shock pressures to form hot spots. Moreover, as the void size increases, the temperature of the formed hot spot increases [12]. Many experiments concluded that the quantity of voids in a material has a strong influence on the shock sensitivity [13]. However, recent advancements in the

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field emphasize on the size of the defect since a larger number of small voids does not have a greater sensitizing effect [14,15]. This paper presents a numerical strategy to computationally investigate problems of this nature.

Hydrocodes based on continuum theories cannot accurately capture the aforementioned processes without numerical modeling. Various models have been used to numerically introduce heterogeneity when simulating shock to detonation transition using an Eulerian approach. Perhaps the most commonly used is the Ignition and Growth Model developed by Lee and Tarver [16], which has shown its ability to accurately represent experimental results for the transition to detonation process from hot spots. The model assumes that a small fraction of the explosive is ignited by the passage of the shock and the reaction growth is controlled by pressure. The formulation consists of several empirical constants, which are calculated through fitting to experimental results with specific configurations. Although the model performs well in simulating the ignition and transition to detonation, it does not predict the effects of the changes in the micro-structure of the material and thus, sensitivity. Other models like the Forest Fire [17] and the JTF (Johnson–Tang–Forest) model [18] have also been successfully implemented. However, these too require experimental *a priori* knowledge of the initial hot spot temperature and its evolution as a function of shock pressure [19]. These models share the same fundamental understanding that a comprehensive knowledge of the spatial and temporal distribution of the energy depositions is required for the proper prediction of the performance and sensitivity of energetic materials [20]. Yet, instead of using a statistical description of the micro-structure, localized energy releases must be modeled through closure models to correctly capture the phenomena at the micro-scale level [21].

Another school of modeling of the shock initiation of explosives seeks a micro-mechanical description of the events leading to hot spot formations. Among these techniques is work by Massoni et al. [22], who distinguish between two classes of models. They refer to the first main class as empirical models built on reaction kinetics with characteristic induction times for the hot spot creation, ignition, and bulk reaction. For example, Ignition and Growth, JTF, and the Forest Fire models are classified in this group. The second main class is referred to as mechanistic models, such as those by Kang et al. [23] and Khasainov et al. [24]. These are based on visco-plastic void collapse models. Massoni's work made use of such models and coupled them with the wave capturing macro-scale through reaction models [22]. Building on this work, Doolan [25] improved its computational efficiency to allow for two-dimensional simulations by reducing the cost of computing induction times. His approach determined induction times from prior visco-plastic simulations and reduced them to an analytical expression, thus eliminating the need to resolve the equations of motion for the gas phase. The present work seeks a computational strategy to efficiently simulate batches of new energetic materials without resorting to the costly experimental process. Therefore, this work adopts a *mechanistic* approach to incorporate hot spot forming mechanisms in a continuum based model, using results from previous sophisticated molecular dynamics and visco-plastic simulations.

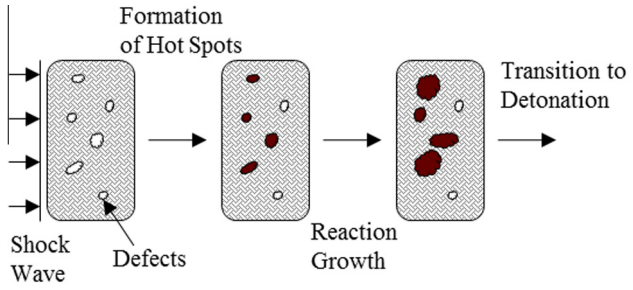

Fig. 1. Schematic of the hot spot formation and transition to detonation process.

Improved prediction of the performance and the sensitivity of energetic materials requires a comprehensive formulation of the complex processes involved. More recent studies have focused on the micro-mechanical and structural processes involved in the formation of hot spots. These include more mechanisms than only visco-plastic heating, which require resolutions at the micro-scale and sometimes at the molecular level. Various computational efforts are geared towards constructing correlations between the material's properties and hot spot formation characteristics [26,27]. In their work, Gilbert et al. [28] used finite and discrete element techniques to provide statistical relationships between the material's structure and hot spot intensity, size, and count. Their studies used HMX packing of different particle sizes to investigate the effects of porosity. Working on Polymer-Bonded Explosives (PBXs), Barua et al. [29] computed the thermal response of various HMX/Estane volume fraction packings as a function of loading conditions. Other studies also incorporated nonlinear elasticity and crystal plasticity in a continuum model to resolve for wave interactions in single crystal PETN [30,31]. Their work identified the different mechanisms involved in activating the primary slip system along various impact orientations. Working on the same problem, Cai et al. [32] made use of molecular dynamics simulations to compute the temperature rise due to grain deformation. Their numerical approach was also utilized to characterize hot spots forming at material interfaces such as those found in PBXs [33,34].

Various studies have successfully captured the hot spot formation mechanisms [33–36], however, their extension to full-scale tests is prohibitively costly. On the other hand, the inclusion of such mechanisms in numerical simulations is critical to ensure reliability in predictions. At this juncture, a model is needed to bridge the gap between the micro-scale and the large scale simulations [37], one that relies on physical and chemical properties. Interest in developing such a model is emphasized in various studies [21,37]. Kapahi and Udaykumar [21] listed key elements that such a model needs to take into account, such as the shock strength, the size of void, the key time scales, and factors that dominate the ignition and the reaction progress. Their work focused on the micro-scale mechanisms involved in the heat released during a void collapse. Using an Eulerian approach, the fluid conservation laws are coupled with deviatoric and plastic strain equations. Their studies track the evolution of the void boundary to capture the localized high temperature regions.

On a larger scale, work by Zhang et al. [37] investigated the transition to detonation process in HMX. Using a hot spot model, their approach initiated detonation with relatively low shock pressures. Their model consisted of a density profile, which is lower at the location of the void, causing a temperature rise behind the shock. The approach successfully increased the sensitivity of a homogeneous material with the flexibility of a density function that can be calibrated to match experiments.

The present paper aims at constructing a mechanistic model to be used in a continuum formulation at the larger scale. Using energy depositions, localized temperature spikes can be achieved. Instead of calibrating to experiments, hot spot formation data are extracted from the results of previous micro-scale and molecular dynamics computations. These provide the means to construct the intensity and induction time parameters, characteristic of the hot spots, as a function of the energetic material's structure and loading conditions. The behavior of the developed model is evaluated in the shock initiation of HMX and PETN, which entertain different hot spot formation mechanisms.