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Research paper

Modeling ignition prediction of HMX-based polymer bonded explosives under low velocity impact

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ABSTRACT

Visco-SCRAM and the hot spot models are applied to predict the ignition of HMX-based polymer bonded explosives (PBXs) under low velocity impact. The model is implemented in the commercial software DYNA3D. The confined Steven test simulation is done to verify the model and to understand the mechanical and thermal response of PBXs. The ignition time as a function of the impact velocity is analyzed. Higher impact velocity results in shorter ignition time. Moreover, the empirical formula is demonstrated to predict the ignition time. Five different dimensions of the specimen ϕ70 mm × 13 mm, ϕ98 mm × 13 mm, ϕ140 mm × 13 mm, ϕ98 mm × 26 mm and ϕ98 mm × 39 mm are applied to obtain the specimen size effect on the ignition. The temperature rise distribution inside the specimen based on the hot spot model and the impact velocity threshold value are successfully predicted. The impact velocity threshold value is in agreement with the experimental data. The velocities 44 m/s, 45 m/s, 45 m/s, 66 m/s and 75 m/s are for the five specimens mentioned above respectively. In addition, the ignition due to different shape projectiles is analyzed. The simulation result shows the impact velocity threshold value is 45 m/s, 97 m/s and 21 m/s for the oval projectile, the flat projectile and the pin projectile respectively. The differences of the temperature rise among the three projectiles are analyzed in detail. In these cases above, the ignition prediction matches experimental results well and the details of mechanical and thermal response of PBXs, such as the deformation of specimens and the temperature rise histories at different positions, are further discussed. Frictional work is considered as the main ignition mechanism of HMX-based PBXs under low impact velocity.

1. Introduction

The ignition of polymer bonded explosives (PBXs) induced by impact has been focused in the past decades (Gibbs and Popolato, 1980). Understanding the mechanism of the ignition phenomenon is important for the manufacture, storage, transportation and usage. The impact-induced ignition is the result of the mechanical response and thermal response of the materials. However, it is difficult to use a single constitutive model to describe the behavior of PBXs due to the complexity of its components and its microstructure (Bardenhagen et al., 2012; Bardenhagen et al., 2006).

The occurrence of ignition highly depends on the characteristic of loading. High speed impact or shock waves can result in the violent reaction of PBXs in the case of pressure pulses of 1–10 GPa and 1–10 microseconds, which is defined a shock to detonation phenomenon (Horie, 2009). By contrast, ignition can also occur in the case of a lower pressure of around 100 MPa and a longer time 1–10 ms, which is known as non-shock ignition phenomenon (Asay, 2010).

Hot spot theory is the main perspective to explain the occurrence of ignition for both shock ignition and non-shock ignition (Bowden and Yoffe, 1985). The mechanism of hot spot formation has been intensively studied. Under shock the hot spot originates from air voids and shear band formation. Classical ignition models, such as Lee-Tarver ignition model and the Kim ignition model, describe the mechanism of shock ignition and match the experiments well (Kim, 1989; Lee and Tarver, 1980). Unfortunately, these models fail in non-shock ignition due to the unknown mechanisms.

In the past decades, a significant amount of experimental investigation on low velocity impact has been conducted to figure out the basic phenomenon and mechanisms of non-shock ignition. American National Laboratories developed a series of standard experiments, such as, Steven test, dropweight test, Susan test and Spigot test (Vandersall et al., 2002; Idar et al., 2001; Chidester et al., 1998; Dorough et al., 1965). Vandersall et al., (2005) measured the ignition impact velocity of different energetic materials in the Steven test. Moreover, Vandersall et al. (2005, 2004) found the projectile shape effect on the ignition

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impact velocity. Niles et al. (2002) applied multi-dimensional gauge techniques to obtain the pressure level and the ignition time in the Steven test. Ma et al. (2013a) discussed the specimen size effect on the ignition impact velocity. The probable microstructure mechanisms, such as damage, friction and plastic deformation, are predicted to play an important role in the non-shock ignition. Chidester et al. (2000) and Idar et al. (2001) demonstrated that a specimen with inner damage could be more sensitive under low velocity impact. Chen et al. (2005) developed a new experimental technique to observe the microstructure morphology of the inside of a specimen and quantified the degree of damage under different impact velocities.

Based on experimental observations, different ignition models have been widely developed. Yang et al. combined elasto-plastic and reactive flow models to describe the mechanical and ignition-deflagration response of PBXs under a low-to-medium-level impact (Yang et al., 2017). The whole model was based on macroscopic phenomenological view. Wu and Huang proposed a micro-mechanics model to predict hot spot formation in energetic crystal powders, considering contact deformation, friction and chemical reaction among the particles (Wu and Huang, 2011). Gruau et al. (2009) modeled the behavior of PBXs by an elastic-plastic-damage law with an ignition criterion due to microstructural plastic strain localization. The simulation result was consistent with experiment. Barua et al. (2013) integrated the thermal ignition criterion with the framework and characterized hot spot fields and hot spot size-temperature. The work demonstrated that this model could be applied for both shock and non-shock ignition.

A classical ignition model is Visco-SCRAM which has been used to predict the non-shock ignition of PBXs. It was first proposed by Bennett et al. (1998). This model considers the viscoelasticity property of PBXs. Interior micro-crack growth was included in the model. This constitutive material model has been well validated (Haberman and Bennett, 1998a, b) and applied to describe the mechanical behavior of PBXs (Xiao et al., 2017; Le et al., 2010). Hot spots form because of the frictional work between two crack surfaces in the microstructure. It has been successfully applied to describe the mechanical behavior and predict ignition of energetic materials (Bilyk, 2006). The methodology can be used as a guide for developing similar models in this field.

The present study implemented the Visco-SCRAM with hot spot model in the commercial software DYNA3D. A typical HMX-based PBX was chosen. Its mechanical and thermal responses in the confined Steven test were discussed for different impact velocities. Moreover, the critical parameter, ignition time, was obtained. Furthermore, the trend of ignition time with velocity was estimated. The influence of the different dimensions of the specimen and different projectile shapes on the ignition was analyzed. More details of the temperature region and hot spot field are shown. These results can help understanding of the ignition mechanism and quantify the ignition phenomenon well under low velocity impact.

2. Constitutive material model and hot spot model

The ignition model includes a constitutive material model and a hot spot model to describe the mechanical behavior and thermal behavior of PBXs. In this section, a brief summary of the model is presented to describe the critical ideas. Full details of the model can be found in the original paper (Bennett et al., 1998). The computational framework is discussed in detail, as it is useful to understand how to implement the model in DYNA3D.

2.1. Constitutive material model

PBXs are highly filled particulate materials, which are bound together by a polymer matrix. Due to the complex heterogeneous structure and the viscoelasticity of the polymer matrix (Mas et al., 2002), PBXs exhibit the viscoelastic mechanical behavior (Heider et al., 2017; Quidot et al., 2000). Therefore, a general n-component Maxwell viscoelasticity material model is applied. The combination of the Maxwell viscoelasticity model with statistical crack mechanics is called Visco-SCRAM (see Fig. 1). The statistical crack mechanics model completely describes the evolution cracking in brittle materials under large deformation has a physical micromechanical perspective (Dienes, 1985).

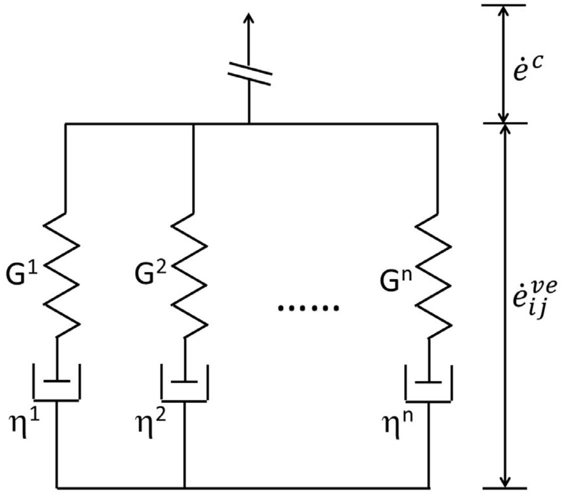

Fig. 1. The constitutive material model: Visco-SCRAM model.

The constitutive material model is described by formulas (1) and (2):

$$\dot{S}_{ij} = \frac{2G\dot{e}_{ij} - \sum_{1}^{N}\frac{S_{ij}^{n}}{\tau^{n}} - 3\left(\frac{c}{a}\right)^{3}\frac{\dot{c}}{a}S_{ij}}{1+\left(\frac{c}{a}\right)^{3}} \tag{1}$$

Where a is the initial flaw size, c is the average crack radius (Addessio and Johnson, 1990), G is the shear modulus, $\dot{e}$ is the deviatoric strain rate, $\dot{S}$ is the deviatoric stress rate and S_{ij}^{n} is the deviatoric stress of the n^th^ Maxwell component.

The deviatoric stress rate of the n^th^ Maxwell component $\dot{S}_{ij}^{n}$ can be expressed as:

$$\dot{S}_{ij}^{n} = 2G^{n}\dot{e}_{ij} - \frac{S_{ij}^{n}}{\tau^{n}} - \frac{G^{n}}{G}\left[3\left(\frac{c}{a}\right)^{2}\frac{\dot{c}}{a}S_{ij} + \left(\frac{c}{a}\right)^{3}\dot{S}_{ij}\right] \tag{2}$$

Where τ^{n} is the relaxation time of the n^th^ Maxwell component, G^{n} is the shear modulus of the n^th^ Maxwell component. Note that in real application, a five-component Maxwell model is used.

In addition, the crack growth rate based on Dienes' work is applied to implement the solution of formula (1) and (2) (Dienes, 1996). The rate is determined by the stress intensity.

$$\dot{c} = v_{max}\left(\frac{K}{K_{1}}\right)^{m} \quad K < K' \tag{3}$$

$$\dot{c} = v_{max}\left[1-\left(\frac{K_{0}}{K}\right)^{2}\right] \quad K \geq K' \tag{4}$$

where $K' = K_{0}\sqrt{1+\frac{2}{m}}$, $K_{1} = K_{0}\sqrt{1+\frac{2}{m}}\left[1+\frac{m}{2}\right]^{\frac{1}{m}}$, $K = \sqrt{\pi c}\,\sigma$, $\sigma = \sqrt{\frac{3}{2}S_{ij}S_{ij}}$, K_{0} is the initial stress intensity factor, m is the factor of the propagation velocity of micro cracks, v_{max} is the maximum propagation velocity. Note that the stress intensity factor K is determined by the crack length and the equivalent stress σ. According to the definition of the equivalent stress, it is calculated by the deviatoric stress.