



# Mesoscale thermal-mechanical analysis of impacted granular and polymer-bonded explosives



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## ABSTRACT

Localized deformation within energetic materials under impact loading may lead to the formation of hot spots, which can cause initiation or detonation of energetic materials. In this work, the thermal-mechanical response of cyclotetramethylene-tetranitramine (HMX) based granular explosives (GXs) and polymer-bonded explosives (PBXs) under impact loading has been investigated using finite element software ABAQUS. A series of three-dimensional mesoscale calculations is performed at impact velocities from 100 m/s to 500 m/s using a crystal plasticity constitutive model for HMX crystals that accounts for nonlinear, anisotropic thermoelasticity and for crystal plasticity. For PBX simulations, a viscoelasticity model is used for the polymer binder. Results show that the average and localized stress and temperature field, which are greatly affected by crystal anisotropy and polymer binder, of GXs are larger than those of PBXs. Qualitative agreement with Pop Plots from the experiments shows that GXs are more sensitive than PBXs.

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## 1. Introduction

The explosive crystals in polymer-bonded explosives (PBXs) are randomly embedded in a polymer binder unlike in granular explosives (GXs), which consist only of compacted explosive crystals. PBXs typically contain 2%–10% (by mass) of polymer, with the remainder consisting of a second explosive, such as cyclotetramethylene-tetranitramine (HMX), cyclotrimethylene-trinitramine (RDX), and pentaerythritol-tetranitrate (PETN). However, prediction of initiation within energetic materials such as GXs and PBXs under impact loading remains a formidable challenge.

Previous studies have shown that a polymer binder has a significant effect on the mechanical properties and sensitivity of PBX explosives (Swallowe and Field, 1982; Williamson et al., 2008), despite their small volume fraction. Bardenhagen and Brackbill (1998) investigated stress bridging and stress fingering in lattices of cylindrical grains using particle and cell computational approach. They found the properties of the binder to be the dominant factor affecting stress distribution and localization in the grains. In

the present study, Estane 5703, a typical binder material in PBX 9501, was chosen to quantify the effects of a polymer binder.

Many studies have been conducted on PBXs to examine the effect of crystal size (Tang et al., 2007), crystal defects (Armstrong et al., 2002; Rae et al., 1998), and binder properties (Cady et al., 2006). Some isotropic models have been proposed to describe the observed mechanical behavior of energetic single crystals and PBXs. Dienes (1996, 1978, 1985) developed statistical crack mechanical model (SCRAM) to account for features such as crack opening and shear in the growth and coalescence of an ensemble of multiple penny-shaped cracks in PBX composites. The developed visco-SCRAM material model has been used to simulate both quasi-static and dynamic behavior. This model has also been validated against several experimental tests (Bennett et al., 1998; Hackett and Bennett, 2000). Baer (2002) and Benson (1999) examined the thermal-mechanical responses of granular HMX under shock loading using Eulerian simulations. A series of Lagrangian simulations on mesoscale behavior to predict ignition has been conducted by Barua et al. (2011, 2012a, b) and Panchadhara and Gonthier (2011). The study of Barua specifically included several dissipative mechanisms, such as fracture and friction, in HMX crystals and a polymer binder using the cohesive finite element method (CFEM). Panchadhara and Gonthier quantified the

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microstructural response in granular explosives and confirmed the importance of plasticity and friction among individual HMX grains in hot spot formation. These studies reported above have analyzed the dissipation mechanisms and thermal-mechanical response of PBX at different scales. However, few analyses have been carried out to account for the crystalline nature of HMX crystals and to study the mechanics of crystal deformation.

Defect-based mechanisms, such as the collapse of pores or voids (Bowden and Yoffe, 1952; Chaudhri and Field, 1974; Field et al., 1992), formation of adiabatic shear bands (Afanas'ev et al., 1972; Winter and Field, 1975), avalanches of dislocation pile-ups (Armstrong et al., 1982; Armstrong and Elban, 2006; Coffey, 1981), and friction of crack surfaces (Bowden and Gurton, 1949; Chaudhri, 1976), have been examined as possible sources of hot spots. However, some experiments results are not well supported by defect-based mechanisms. For example, initiation sensitivity of defect-free PETN single crystals and HMX single crystals is observed to depend strongly on crystalline orientation (Dick, 1984, 1997; Dick et al., 2004; Dick et al., 1991; Dick and Ritchie, 1994; Menikoff et al., 2005).

In order to explain the anisotropy in shock initiation, a steric hindrance model was developed to explain the observed anisotropic deformation pathways and the sensitivity to shock initiation of PETN (Dick and Ritchie, 1994, 1997). Furthermore, researchers examined the crystal plasticity model accounting for dislocation mobility at the subgrain scale to explain the orientation-dependent behavior of energetic single crystals (Barton et al., 2009; Hardin et al., 2014; Rimoli et al., 2010; Wu and Huang, 2012a). Rimoli et al. (2010) developed a 3D Lagrangian framework to analyze the thermal-mechanical responses of PETN by regarding crystal plasticity as the only dissipation mechanism, and Hardin et al. (2014) investigated the thermal-mechanical response of polycrystalline HMX based on this framework. Barton et al. (2009) adopted the crystal mechanic-based model, and Austin (2015) incorporated decomposition reactions to study the pore collapse and ignition of  $\beta$ -HMX under shock loading. In our work, the dislocation-based crystal plasticity model has been used for HMX crystal and anisotropy behavior has been considered.

In practice, explosives are more likely to be subjected to low pressure impact loading conditions, where XDT often occurs. In the present study, we assume anisotropic crystal plastic slip and volumetric work are dominated by dissipation mechanisms rather than by fracture and friction. Although this is an idealization, it makes quantifying the dislocation-based crystal plasticity mechanism much easier not to consider such other factors as fracture and void collapse. HMX crystals are the main constituents in several PBXs and GXs. Although HMX is a polymorphic crystal with  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  polymorphs depending on temperature and pressure.  $\beta$ -HMX, which is the most stable structure at room temperature (Menikoff and Sewell, 2002), is considered in this study. Sheen et al. (1993) reported operative slip systems in  $\beta$ -HMX,  $(001) < 100 >$  and  $(101) < 10\bar{1} >$  based on the monoclinic crystallographic axis (a, b, and c) in space group P2<sub>1</sub>/n.

The present paper has two main objectives: (i) to investigate the effect of crystal anisotropy and microstructural heterogeneity on mesoscale thermal-mechanical responses of GXs and PBXs based on a crystal plasticity model and (ii) to quantify the interaction between an anisotropic crystal phase and an isotropic polymer binder phase under different impact velocities from 100 m/s to 500 m/s. In this work, each  $\beta$ -HMX crystal in GXs and PBXs has the same crystal orientation, crystal size, and morphology to ensure that the effect of polymer binder is the only factor determining the differences in the microstructural responses. Moreover, each HMX single crystal is assigned a distinct dislocation-based rate-dependent constitutive model to take nonlinear elasticity and anisotropy into consideration. As such, stress and tempera-

ture fields are evaluated for the anisotropy of the crystals and for microstructural heterogeneity.

## 2. Theory and constitutive models

In this section, a brief outline is presented of the thermal mechanical constitutive model for HMX crystals. The model used herein follows that developed by Wu and Huang (2010) to interpret the planar impact experiments on HMX single crystals by Dick et al. (2004). The development extends earlier work on crystal plasticity (e.g. Hill and Rice, 1966; Asaro and Rice, 1977; Peirce et al., 1983; Asaro, 1983a, b; Asaro and Needleman, 1985; and Ortiz et al., 2001) to cases where modeling of response at high pressure is considered.

### 2.1. Slip system kinetics and dislocation-based crystal plasticity

Based on the standard multiplicative decomposition, the deformation gradient can be represented as  $F = F^e F^p = R^e U^e F^p$ . In this decomposition,  $R^e$  denotes the crystalline lattice rotation,  $U^e$  denotes the crystalline lattice stretch and  $F^p$  denotes the plastic deformation, which in the deformed, but unrotated configuration, can be represented as

$$\bar{F}^p = U^e F^p \quad (1)$$

Plastic deformation of a crystal is assumed to be related only to dislocation motion on crystalline slip systems, so that

$$\bar{L}^p = \dot{\bar{F}}^p \bar{F}^{p-1} = \sum_{\alpha=1}^N \dot{\gamma}^\alpha (\bar{s}^\alpha \otimes \bar{m}^\alpha) \quad (2)$$

where  $\bar{s}^\alpha$  and  $\bar{m}^\alpha$  are the slip direction and the slip plane normal respectively, in the deformed but unrotated configuration  $\bar{B}$ .  $\dot{\gamma}^\alpha$  is the shear strain rate on slip system  $\alpha$ .

In order to characterize the rate dependent crystal plasticity, the Orowan equation (Gilman, 1969) is adopted

$$\dot{\gamma}^\alpha = \rho_m^\alpha b^\alpha \bar{v}^\alpha \quad (3)$$

where  $b^\alpha$  is the Burgers vector,  $\rho_m^\alpha$  is the mobile dislocation density and  $\bar{v}^\alpha$  is the average dislocation velocity on slip system  $\alpha$ .

Dislocation velocity is assumed to be related to resolved shear stress  $\tau^\alpha$  as (Gupta et al., 1975),

$$\bar{v}^\alpha = v_0^\alpha \exp \left[ \frac{-s_d}{(\tau^\alpha - \tau_0)} \right] \quad (4)$$

where  $v_0^\alpha$  is the shear wave velocity,  $s_d$  is a drag stress,  $\tau_0$  is the threshold shear stress for dislocations motion. Initially the dislocation velocity increases slowly after resolved shear stress  $\tau^\alpha$  exceeds  $\tau_0$  followed by a rapid increase at about  $s_d/2$ . The dislocations are limited to move at velocities less than the shear wave velocity for the corresponding shearing direction.

Two distinct processes contribute to the strain rate: nucleation of dislocation loops and growth of existing loops (Hull and Bacon, 1984). At low strain rates, increases in dislocation density are usually attributed to multiplication of existing dislocations via a process called multiple cross glide (Gilman and Johnston, 1962). On the other hand, for solids under extremely large shear stresses the nucleation of dislocations at stress concentrations must be considered (Hirth and Lothe, 1982). At higher stresses, the nucleation and multiplication of dislocations will operate simultaneously.

Then, the rate of change of dislocation density can be expressed as,

$$\dot{\rho}_m^\alpha = M \dot{\gamma}^\alpha \exp(-H \bar{\gamma} / \tau^\alpha) + A (\tau^\alpha - \tau_c) \dot{\gamma}^\alpha \quad (5)$$

where  $\bar{\gamma}$  denotes the total cumulative shear strain on each slip system;  $\tau_c$  is a threshold stress for nucleation;  $M$  and  $A$  are material constants.

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