Effects of HMX Particle Size on the Shock Initiation of PBXC03 Explosive

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Abstract. A series of shock initiation experiments are performed on the PBXC03 explosives in different formulations to understand the influence of the explosive particle size on the shock initiation, and the in-situ pressure gauge data are obtained which show that shock sensitivity decreases with the explosive particle size under the test condition used in this paper. Moreover, a mesoscopic reaction rate model which is calibrated by the experimental data on a medium formulation PBXC03 explosive is adopted and then applied to predict numerically the shock initiation of other PBXC03 explosives in different formulations. The numerical results are in good agreement with the experimental data.

Keywords. Shock initiation, microstructure parameters, particle size effect, mesoscopic reaction rate model.

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1 Introduction

The understanding of the shock initiation and the subsequent detonation growth process of explosives is crucial in the detonation physics, which provides much useful information for the evaluation of the explosive safety and reliability. The microstructure parameters of explosives such as the particle size, the loading density/porosity of charge, the strength and the concentration of the binder are the important factors affecting the shock sensitivity and the sustained

reaction of explosives. Over the past decades, many sensitivity experiments [1–4] such as the gap-test and the wedge-test, etc. have been carried out to investigate the effect of the microstructure parameters on the shock sensitivity of explosives. However, the study on the detonation growth process behind the shock wave focuses mainly on the effect of loading pressure, confinement conditions and temperature [5–9] by the experimental method using the in-situ manganin pressure gauges and the numerical method using Ignition and Growth reactive flow model, and there are few people to care about the difference of detonation growth progress for the explosives with different microstructures.

Moreover, due to the limitation of the traditional empirical models such as Forest Fire model [10], Ignition and Growth model [11] and JTF model [12], etc., it is hard to reproduce these microstructure effects on the shock initiation of explosives so that some theoretical models have been proposed. For example, Hamate and his co-workers [13,14] developed a micromechanical burn model to describe the influence of the average size of the explosive particles by using a parameter related to the specific surface area of the explosive particles, and the derived Pop-plot curve is in substantial agreement with the experimental data presented by Khasainov et al. [2]. The present authors developed a mesoscopic reaction rate model [15] to describe the effects of the microstructure parameters of explosives including particle size, porosity, the strength and the concentration of the binder on the shock initiation.

In this paper, shock initiation experiments by the in-situ manganin piezoresistive pressure gauge technique are carried out to investigate the influences of the HMX particle size on the shock initiation and the subsequent detonation growth process of the pressed PBXC03 (87% HMX, 7% TATB, 6% Viton by weight) explosive. Moreover, to investigate theoretically in more details the above mentioned microstructural effects, a kind of mesoscopic reaction rate model [15] is adopted to simulate numerically the shock initiation, and the numerical results is found to be in good agreement with the experimental data.

2 Experimental Procedure

The one-dimensional Lagrangian system used for the shock initiation experiment in the study is as shown in Figure 1.

In the experiments, a high-pressure plane detonation wave created by using an explosive plane-wave lens having

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Formulation Identification	composition	Weight %	Volume %	Loading Density (g/cm ³)	TATB Average Particle Size (μm)	HMX Particle Size Range (μm)
Fine	HMX	87	85.58	1.849	15	20–30
Medium	Binder	7	6			70–90
Coarse	TATB	6.76	7.66			110–130

Table 1. PBXC03 Formulations with different particle sizes.

Figure 1. The one-dimensional Lagrangian experimental system.

a diameter of 60 mm and a TNT booster having a diameter of 60 mm and a height of 20 mm is attenuated into a plane shock wave of required intensity by adjusting both the air-gap and the Al-gap of different thickness. The plane shock wave can then be utilized to initiate the PBXC03 explosive, which consists of three thin discs each having a diameter of 50 mm and a thickness of 3, 4 or 5 mm, respectively, and a thick disc having a diameter of 50 mm and a thickness of 25 mm. The third thin disc and the thick disc are stacked to place in the region where detonation is expected. The pressure histories at four different Lagrange locations are measured in every shot experiment. Four gauge packages containing manganin piezoresistive pressure gauges are placed on the top of each thin disc and the thick disc, respectively. The first gauge and the last three gauges are armored by Teflon insulation film having a thickness of 0.2 and 0.1 mm, respectively, on both sides to prevent short circuit of the gauges in a conductive medium when the explosive becomes reactive. A high speed constant-current sync-source is used to supply the needed power for these gauges, and the oscilloscope recorded gauge voltage temporal curve can be converted into the pressure one by using the corrected calibration curve. In addition, the pressure-resistance relation of these gauges used in this paper is as

Figure 2. Photograph of a typical shock initiation experiment driven by the explosive detonation.

follows:

$$P = 0.62248 + 35.20079 \times \frac{\Delta R}{R_0} + 7.68603 \times \left(\frac{\Delta R}{R_0} \right)^2. \quad (1)$$

Where $\Delta R/R = \Delta V/V$, R and ΔR are the gauge resistance and the change of resistance caused by the pressure, respectively; V and ΔV are the gauge voltage and the change of voltage recorded by oscilloscope, respectively.

In order to study the explosive particle size effect, three kinds of the PBXC03 formulations with the same loading density (1.849 g/cm³) are prepared. The composition, loading density and range of particle size of the three PBXC03 formulations are presented in Table 1.

The only variable parameter is the particle size of the HMX crystalline explosive. It should be noted that in the study only the HMX particle size effect is taken into account considering that the PBXC03 formulation contains a little TATB explosive. The Figure 2 shows the photograph of a typical shock initiation experiment driven by the explosive detonation.

3 Experimental Results and Discussion

The measured pressure versus time histories at the four embedded gauge for the PBXC03 formulations with different

Figure 3. Measured pressure histories in the fine formulation PBXC03 explosive.

Figure 4. Measured pressure histories in the medium formulation PBXC03 explosive.

Figure 5. Measured pressure histories in the coarse formulation PBXC03 explosive.

Figure 6. Shock front trajectory for different formulation PBXC03 explosives.

Figure 7. Pressure growth process of shock front for different formulation PBXC03 explosives.

particle sizes are presented as shown in Figure 3 to Figure 5. It can be seen that the growth of the pressure behind the shock front in the fine formulation is much faster than that in the medium and the coarse formulations at the corresponding gauge locations such as 0 and 3 mm. Detonation in the fine formulation explosive occurs before the 6 mm gauge depth, and that in the medium one forms essentially at the 9 mm gauge depth, while, in the coarse formulation explosive, the transition to detonation does not complete yet at the 9 mm gauge depth.

The measured propagation trajectory and the pressure growth process of the shock front in different formulation PBXC03 explosives are shown in Figure 6 and Figure 7, respectively. It is found that as the particle size increases,

$T_0 = 298 \text{ K}$; $\rho_0 = 1.849 \text{ g/cm}^3$; Shear Modulus = 0.0352 Mbar; Yield strength = 0.002 Mbar			
Un-reacted JWL	Product JWL	Reaction rates parameters	
		The first term	The second and third terms
$A = 272137.59 \text{ Mbar}$	$A = 10.2545 \text{ Mbar}$	$Z = 5.0\text{E}+13 \text{ } \mu\text{s}^{-1}$	$a_1 = 0.0073078$
$B = -0.738544 \text{ Mbar}$	$B = 0.2257 \text{ Mbar}$	$T^* = 26500 \text{ K}$	$n_1 = 1.86646$
$R_1 = 19.87$	$R_1 = 14.91$	$C_p = 1.4\text{E}-5 \text{ cm}^2/\mu\text{s}^2/\text{K}$	$G = 2244.06$
$R_2 = 1.987$	$R_2 = 21.37$	$k_e = 8\text{E}-5 \text{ Mbar}$	$Z = 3.322$
$\omega = 1.99$	$\omega = 0.29$	$Q = 5.439\text{E}-2 \text{ cm}^2/\mu\text{s}^2$	$x = 1.82$
$C_V = 1.6932\text{E}-4 \text{ Mbar/K}$	$C_V = 1.0\text{E}-4 \text{ Mbar/K}$	$k^* = 8.0\text{E}-14 \text{ cm}/\mu\text{s/K}$	
	$E_0 = 0.1 \text{ Mbar}$	$k_b = 8\text{E}-5 \text{ Mbar}$	

Table 2. Parameters in equation of state and reaction rate model for PBXC03 [16].

the increase of both the velocity and the pressure of shock front become slow, because that the formulations with the finer particle have larger specific surface areas, and then hot-spots can grow more rapidly. Thus, the run time to detonation is the shortest for the fine formulation explosive, followed by the medium and then the coarse one, and the fine formulation explosive is the most sensitive.

4 Reactive Flow Modeling

To perform the numerical simulation on the shock initiation processes, the two-dimensional hydrodynamics code DYNA2D is used in this paper, together with the mesoscopic reaction rate model [15] in the following form:

$$\frac{d\lambda}{dt} = \frac{d\lambda_h}{dt} + \frac{3\lambda^{2/3}}{r_o} a_1 p^{n_1} + G p^z (1-\lambda)^x, \quad (2)$$

where a_1 , n_1 , G , z and x are all constants, which are determined by the experimental data on shock initiation. The reaction rate model consists of a hot-spot ignition term, a slow-burning term and a high-pressure reaction term, and can be used to describe the effects of microstructure parameters on the shock initiation of PBX explosives.

The hot-spot ignition term can be written as:

$$\begin{aligned} \frac{d\lambda_h}{dt} &= \int_{r_m}^{r_o} \frac{d\Lambda}{dt}(r, x, t) 4\pi r^2 \frac{4}{3}\pi(r_o^3 - r_m^3) dr \\ \frac{d\Lambda(r, x, t)}{dt} &= (1-\Lambda)Z \exp\left(-\frac{T^*}{T(r, x, t)}\right) \\ T(r, x, t) &= T_0(r, x, t) + \int_0^t \frac{dT(r, x, t)}{dt} dt \\ \frac{dT}{dt} &= \left(\frac{dT}{dt}\right)_{M.D.} + \frac{1}{\rho C_p} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 k^* \frac{\partial T}{\partial r} \right) \\ &\quad + \frac{Q}{\rho C_p} \frac{d\Lambda}{dt} \end{aligned}$$

$$\begin{aligned} \left(\frac{dT}{dt}\right)_{M.D.} &= \left(\frac{3\gamma_e \gamma_b^2 k_e}{2\rho C_p}\right) \\ &\times \frac{\left(P_0 - P_g - 2\sqrt{3}k_b \ln \frac{r_m}{r_i} - 2\sqrt{3}k_e \ln \frac{r_o}{r_m}\right)^2}{[(r_o^{-3} - r_m^{-3})\gamma_b k_e + (r_m^{-3} - r_i^{-3})\gamma_e k_b] 2r^6}, \end{aligned} \quad (3)$$

where $\Lambda(r, x, t)$ is the local degree of reaction; Z is the pre-exponential factor in Arrhenius kinetics; T^* and T_0 are the activation and the initial temperature, respectively; k^* is the thermal conductivity; C_p is the heat capacity, and Q is the reaction heat of explosives; γ_e and γ_b are constants related to the explosive and the binder respectively; k_e and k_b are the shear yield strength of the explosive and the binder, respectively. All these parameters are known and associated with the nature of explosive. In addition, the parameters, r_o , r_i and r_m are the microstructure parameters of explosives. Thereinto, r_o is the average radius of explosive particles; r_i is the average pore radius of explosive, which can be derived by

$$\alpha_1 = \frac{r_i^3}{r_o^3} = 1 - \frac{\rho}{\rho_T}, \quad (4)$$

where α_1 , ρ_T and ρ are, respectively, the porosity the theoretical density and the initial density of explosives. The parameter r_m is dependent on the content of the binder in the explosive and can be determined as following

$$\alpha_2 = \frac{V_B}{V_E} = \frac{r_m^3 - r_i^3}{r_o^3 - r_m^3}, \quad (5)$$

where V_B and V_E are the volume of the binder and the explosive, respectively.

The isotropic elastoplastic hydrodynamic model is used for the PBXC03 explosives, in which two Jones–Wilkins–Lee (JWL) equations of state are used; one for the un-reacted explosive the other for the reaction products, in the form:

$$p = Ae^{-R_1 V} + Be^{-R_2 V} + \omega C_V T/V, \quad (6)$$

where p is the pressure in Mega bars; V and T are the relative volume and temperature, respectively; ω is the Grüneisen coefficient; C_V is the average heat capacity, and A , B , R_1 , and R_2 are constants. The un-reacted equation of state is fitted to the available shock Hugoniot data, and the product equation of state is fitted to cylinder test.

The parameters in the reaction rate model and the equation of state for the PBXC03 are listed in Table 2 [16]. The parameters of the second and third terms in reaction rate equation, i.e., a_1 , n_1 , G , z and x , are determined by in-situ pressure gauge data of the medium formulation PBXC03 explosive derived in this paper.

In order to compare the numerical results with the experimental data, the measured pressure temporal curve on the top of the explosive (i.e. at the 0 mm gauge depth) is taken as the computational boundary condition to initiate the explosive. Both the numerical results and the experimental data on the gauge records for the three kinds of PBXC03 formulation are presented as shown in Figure 8 to Figure 10. It can be seen, for the fine PBXC03 formulation explosive that the numerical results are in good agreement with the experimental data, but there are some differences for the medium and coarse PBXC03 formulation explosives. The reason should be that only one kind of ignition mechanism of hot-spot has been taken into account in the reaction rate model, which is too simple to describe so complex scenarios of formulation of the detonation wave. However, the tendency of variation of the growth process of detonation with the particle size of explosive agrees with the experimental data.

The shock initiation experiments driven by the explosive detonation are complex, and it is hard to ensure that the input conditions of every experiment are completely consistent. Therefore, flyer plate impact experiments, which can ensure the consistency of loading conditions through governing the velocity of the flyer plate, are simulated to obtain the shock initiation data of PBXC03 formulation with different particle sizes.

The isotropic elastoplastic hydrodynamic model and the Grüneisen equation of state are used for the aluminum flyer, and the parameters are listed in Table 3.

Figure 11 shows the numerical result for the propagation trajectory of the shock front in the case of that the aluminum flyer impacting the PBXC03 formulations at a velocity of 845 m/s. Comparing Figure 11 with Figure 6 shows that the numerical results have the same trend as the experimental data, which confirms that the mesoscopic reaction rate model used in this paper is reasonable to describe the effects of the microstructure on the shock initiation of the PBX.

5 Conclusion

Shock initiation experiments using the in-situ manganin piezoresistive pressure gauge technique are performed on

Figure 8. Numerical results and experimental data on the pressure histories in fine formulation PBXC03 explosive.

Figure 9. Numerical results and experimental data on the pressure histories in medium formulation PBXC03 explosive.

Figure 10. Numerical results and experimental data on the pressure histories in coarse formulation PBXC03 explosive.

Material model parameters	G (Mbar)	1.07
	σ (Mbar)	0.0044
Grüneisen parameters	ρ_0 (g/cm ³)	2.785
	C (cm/ μ s)	0.8724
	S_1	0.975
	S_2	0
	S_3	0
	γ_0	1.32
	a	0

Table 3. Material parameters and Grüneisen equation of state parameters used for the aluminum flyer plate.

Figure 11. Computational propagation trajectory of the shock front for PBXC03 formulation with different particle sizes.

the PBXC03 explosives in three different formulations, namely, the fine, the medium and the coarse one, under the same loading conditions. It is shown that the run distance to detonation is the shortest for the fine formulation explosive, followed by the medium and then the coarse one, and the fine formulation explosive is the most sensitive under the test conditions used in this paper.

The parameters of the mesoscopic reaction rate model are obtained to fit the in-situ pressure gauge data on the medium formulation PBXC03 explosive, which is utilized to predict the shock initiation behavior of the other PBXC03 explosives in different formulations. The numerical results are in good agreement with the experimental data derived in this paper, which are also coincide with the previous experimental results presented by Khasainov et al. [2] as well as the numerical results obtained by Hamate [13].

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