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Numerical Study on Deformation and Ignition Process of Impacting Granular HMX Explosive in Drop Hammer Test

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Abstract: Two-dimensional numerical simulation of the impact process for drop hammer on granular HMX was carried out by using ANSYS/AUTODYN software. The temperature rise generated in particles was estimated via the principle converted from plastic work to heat energy based on the calculated values of stress and plastic work. The HMX particles was geometrical shapes and round, assuming that the particles had elastic-plastic deforming properties. Particle stack form had two kinds of situations of regular and irregular arrangement. The initial velocity of the drop weight was calculated through setting the drop height and the formula of free fall. For different drop heights and the calculation of different yield stress values of sample particle material, the temperature rise changes in particles under drop hammer impact were obtained. The results showed that the regular arrangement produces low temperature (37.2 °C) rise, whereas the irregular arrangement produces higher temperature (142.9 °C) rise. In irregular arrangement, the local plastic deformation work of particles can lead to higher temperature rise, causing particle ignition. At the same time, considering the uncertainty of the yield stress value of HMX, the calculation of temperature rise is performed taking the smaller yield stress value (0.13 GPa), while the other calculation conditions are the same, and the temperature rise obtained is 83.2 °C, which got 59.7 °C lower than the yield stress value of 0.26 GPa.

Key words: drop hammer test; HMX particles; numerical simulation; temperature rise

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1 Introduction

Drop hammer apparatus is widely used to test the impact sensitivities of energetic materials. Until present, there is just a little research work toward the quantitative analysis for the ignition process in the tests. Experimentally, Bowden and Yoffe^[1] conducted drop hammer test and first proposed the concept of hot spots inside explosive under impact. They thought that the internal gas adiabatic compression, crystal surface frictions and viscous heat caused by turbulence are the main reasons for hot spot formation. Field^[2] modified drop hammer test equipment to get the detailed knowledge of hot spot formation. Through observations, he concluded that the adiabatic bubble temperature, adiabatic shear band and surface or the internal friction are the main reasons for the ignition of explosives. Considering the factor of the grain effectiveness, Gonthier^[3] studied the compaction ignition process using impact speed from $10 \text{ m} \cdot \text{s}^{-1}$ to $100 \text{ m} \cdot \text{s}^{-1}$. He studied the effect of viscous elastic-plastic contribution to the ignition in grain explosives. Yushi Wen et al^[4] conducted a drop weight tests on three samples including crystal powders of RDX, tetryl, and PBX powder to probe the correlation between the ex-

plosion probabilities and the sample dose. And they found that the explosion probability will firstly increase and then decrease when the mass of sample reduces from 50 mg to 1.1 mg, under drop height of 25 cm and a 10 kg hammer. They explained the increasing part by proposing that the less mass the more energy the explosive sample absorbs and the easier the explosions occur, leading to higher explosion probability. The other part is a little complicated, they used a dual-factor-competition model to explain in their paper. To a block of PBX-9501 explosive (plastic bonded explosives with HMX mass fraction of 95%) under the impact with a medium speed, Bennett^[5] simulated the dynamic response of impact test by using the DYNA3D software. He revealed that the main ignition mechanism is due to the friction on the shear fracture surfaces. However, it is difficult to present the hot spot formation and the meso-size process development owing to the small size of the hot spot (0.1–100 μm magnitude) and the short time to ignition (0.1 μs magnitude). In this paper, we utilize the numerical simulation method to study the deformation processes of explosive particles under the low-speed ($<10 \text{ m} \cdot \text{s}^{-1}$) impact of drop hammer in the practical drop hammer device. The plastic energy in the particles was investigated to examine its role in the formation of hot spots in HMX explosive. The temperature rises in HMX particles were calculated and compared with the critical ignition temperature from other experimental measurement.

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2 Numerical Simulation

2.1 Brief Description of Drop Hammer Apparatus

Drop hammer apparatus is a device to be utilized to measure the impact sensitivity of explosives as shown in Fig. 1. The hammer drops along a guide rail. From a certain height, the hammer falls freely and hits on the striker. The explosive material is placed between the striker and the anvil. The drop hammer, striker, anvil, guide sleeve and the base are generally made of steel cylinders. Fig. 2 illustrates the tester part of the device in detail. Our simulation model will be established from it.

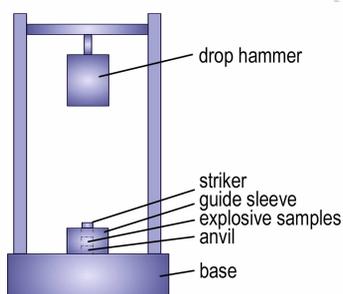


Fig. 1 Schematic diagram of drop hammer apparatus

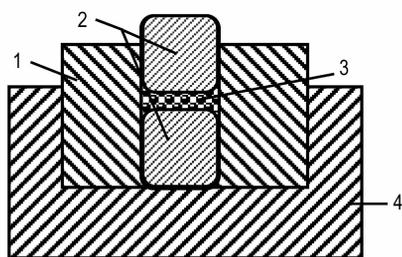


Fig. 2 Schematic diagram of impact tester
1—guide sleeve, 2—strikers, 3—explosive samples, 4—base

2.2 Computational Model

Based on the actual drop hammer apparatus, it is assumed that the hammer directly impacts onto the striker with an initial speed. The stresses and strains in the striker, particles, the hammer and the anvil are investigated. The computational model system consists of drop hammer, striker, anvil, guide sleeve and explosives particles. The ANSYS Design Modeler software is employed to draw the computational shapes of the components given in Fig. 2. The gained configuration is shown in Fig. 3. The configuration in simulation contains five parts of drop hammer, striker, HMX particles, anvil, and guide sleeve. In the calculations, the anvil and the guide sleeve are assumed to be stationary. Area-1 in Fig. 3 is the location of the HMX particles and the detailed particle distribution is amplified in Fig. 4. The dimension of HMX particle is chosen from the practical characteristic scale size. For the computational conven-

ience, the shape of the particle is simplified as a circle. The particles are evenly stacked in layer by layer. There are 25 particles at the bottom layer in half of the configuration (Fig. 4). Considering the fact of the symmetry of the model, half of the configuration is selected to calculate during simulation.

In the model, both the diameters of striker and anvil are 10 mm and their heights are 10 mm. The outer diameter of guide sleeve is 40 mm, the inner diameter is 10 mm and the height is 16 mm. The drop hammer is 5 kg, the diameter is 40 mm and the height is 127 mm. The HMX particles have single diameter of 200 μm. The materials steel and HMX follow an elastic-plastic deforming behavior. Their materials parameters are listed in Table 1 and Table 2, respectively.

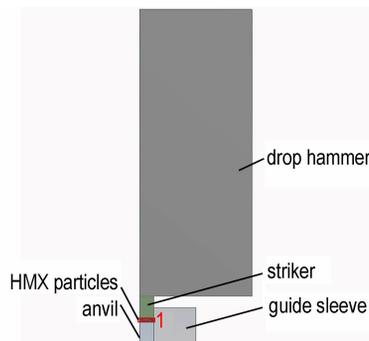


Fig. 3 Simulation diagram of impact structure (1-sample area)

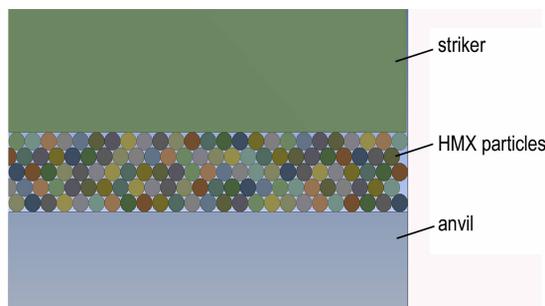


Fig. 4 The amplification of impact structure schematic diagram

Table 1 Parameters of steel material^[6]

material	density /kg · m ⁻³	elastic modulus /GPa	specific heat capacity /J · kg ⁻¹ · K ⁻¹	yield strength /GPa	Poisson ratio
steel	7830	210	460	0.31	0.30

Table 2 Material parameters of HMX^[3]

material	density /kg · m ⁻³	elastic modulus /GPa	specific heat capacity /J · kg ⁻¹ · K ⁻¹	yield strength /GPa	Poisson ratio
HMX	1903	24.0	1500	0.26 ^[6] /0.13 ^[7]	0.20

In the experimental tests for HMX particle samples, it is found that using 5 kg hammer the impact drop height H_{50} is

33 cm, from which letting the hammer fall, the probability of the ignition occurs is about 50%. According to this data, in the simulation, H_{50} is used to get initial velocity for drop hammer. The velocity is calculated to be $2.543 \text{ m} \cdot \text{s}^{-1}$, at which the hammer will hit the striker. Accounting for the influence of the gravity, the system is subjected to the gravitational acceleration of $9.806 \text{ m} \cdot \text{s}^{-2}$. In the calculation, the time step is automatically controlled by the program, roughly being $3.1 \times 10^{-10} \text{ s}$.

Assuming that the HMX particles are suitable for the elastic-plastic constitutive model and the simulation uses the dynamic software AUTODYN in the ANSYS products. Before the calculations, the model needs to be meshed. The quadrilateral mesh is used for all parts of the model system. The HMX particles are meshed by general quadrilateral with the characteristic length of $1.5 \text{ } \mu\text{m}$. The other parts are of a square grid, with a typical size of $40 \text{ } \mu\text{m}$. Fig. 5 shows the overall grid partition of the impact system. For the sake of better viewing, Fig. 6 gives a magnification of the mesh of HMX particles.

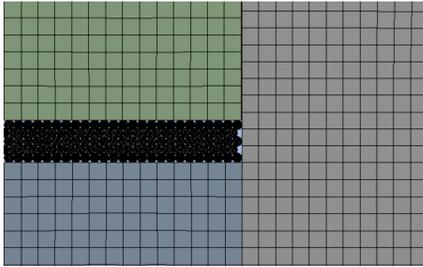


Fig. 5 Mesh partition diagram of impact structure



Fig. 6 Magnification of mesh of HMX particles

3 Results and Discussions

3.1 Calculation Method of Temperature Rise

Since the simulation software does not provide a package for calculating the temperature rise accompanying the deformation, we have to establish a method to calculate it using the stresses and strains obtained from simulation. We already know that the deformation of HMX particles under stress including elastic and plastic deformations. However, the elastic behavior does not produce work to cause temperature rise, so we only discuss the calculation method of plastic work. The calculation formula for plastic work is according to Eq. (1).

$$W_s = \int \sigma d\varepsilon \quad (1)$$

Where σ is the stress, MPa, ε is the strain. In calculating plastic work, an approximate method is taken. Since the stress and the strain are known at any time from the simulation results, the equivalent stress and the equivalent strain at each time can be calculated. The product of these two terms can be thought as equivalent plastic work. Summing the equivalent plastic work at all time phases, the total plastic work is obtained. At each time phase, the averaging stress is calculated according to Eq. (2).

$$\sigma_i^* = \frac{(\sigma_i + \sigma_{i-1})}{2} \quad (2)$$

Where subscript i denotes the time sequence; σ_i^* , MPa, is the average value of the stress of the specific element at the two adjacent time-steps of Δt_{i-1} , μs , and Δt_i , μs ; σ_i , MPa, is the stress of specific element at time-step Δt_i . The initial stress is taken to be $\sigma_0 = \sigma_y$. The variation of plastic strain corresponding to the two adjacent time-steps of Δt_{i-1} and Δt_i is

$$\Delta \varepsilon_i = \varepsilon_i - \varepsilon_{i-1} \quad (3)$$

Where ε_i is the difference of two plastic strains between two adjacent time-steps of Δt_{i-1} and Δt_i ; ε_i is the plastic strain at time-step of Δt_i . In the beginning of the calculation, let $\Delta \varepsilon_0 = 0$. The total plastic work is gained by Eq. (4).

$$W = \sum_{i=1}^n (\sigma_i^* \cdot \Delta \varepsilon_i) \quad (4)$$

Where $W(J)$, is the work done during the plastic deformation of some specific element in all time-steps Δt_1 to Δt_n . n is the number of the computational cycles from the beginning to the desired termination.

Setting the area of the specific element as unit value, the heat is transformed by the partial plastic work $W_s(J)$. We assume that the total plastic work is converted into heat energy, denoted by $Q_s(J)$. And $C_v(J/(kg \cdot K))$ is the volumetric specific heat of HMX material. The temperature rise $\Delta T(^{\circ}\text{C})$, due to the accumulation of heat can be determined by the following Eq. (5).

$$\Delta T = \frac{Q_s}{C_v \rho} = \frac{W_s}{C_v \rho} \quad (5)$$

3.2 Effect of HMX Particle Inhomogeneity on Temperature Rise

In order to investigate the effect of particle inhomogeneity on the local heat formation, the arrangement of HMX particles are constructed into two cases; regular arrangement in which all particles are of the same circular shape and irregular arrangement in which at some locations there are replacements by smaller particles. Furthermore, owing to the fact that there is ambiguity on the yield strength value for HMX particle, two yield strength values are considered. Dick and Menikoff^[7]

gives a 0.26 GPa value by tests, however, Palmer and Field^[8] present the value of 0.13 GPa. At first, a 0.26 GPa value for yield strength of HMX is used in the calculations to analyze the effect on temperature rise for both regular and irregular particle arrangements.

Firstly, we carry out simulations on the case of the regular arrangement. In the calculation of the plastic work, the plastic stress and plastic strain are two important physical variables. Those values should be correctly obtained and kept. Fig. 7 shows stress distribution in HMX particles at $t = 25 \mu\text{s}$, $t = 50 \mu\text{s}$, $t = 75 \mu\text{s}$ and $t = 100 \mu\text{s}$, for the knowledge of the changing process of the particles stress. In Fig. 7, the different colors represent different ranges of the stress magnitude (unit-MPa). Fig. 8 shows plastic strain diagram of HMX particles correspondingly at $t = 25 \mu\text{s}$, $t = 50 \mu\text{s}$, $t = 75 \mu\text{s}$ and $t = 100 \mu\text{s}$. Here, the colors represent different ranges of the plastic strain magnitude. After impacted by the drop hammer, the particles still keep the original regular arrangement, but, the forces in particles are uneven. As time reaches $100 \mu\text{s}$, there appears a location with the maximum of plastic work in the particle system. With yield strength of 0.26 GPa, the location designated as M_1 presents the maximum plastic work just as shown in Fig. 7 and Fig. 8. Fig. 9 shows the varying curves of the local stress and plastic strain with time correspondingly.

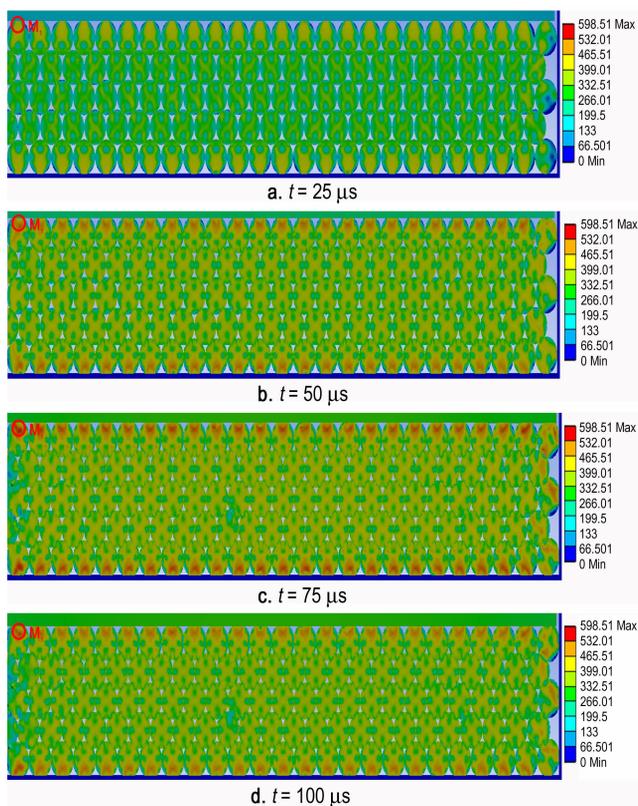


Fig. 7 Equivalent stress of HMX particles at different times in case of regular arrangement

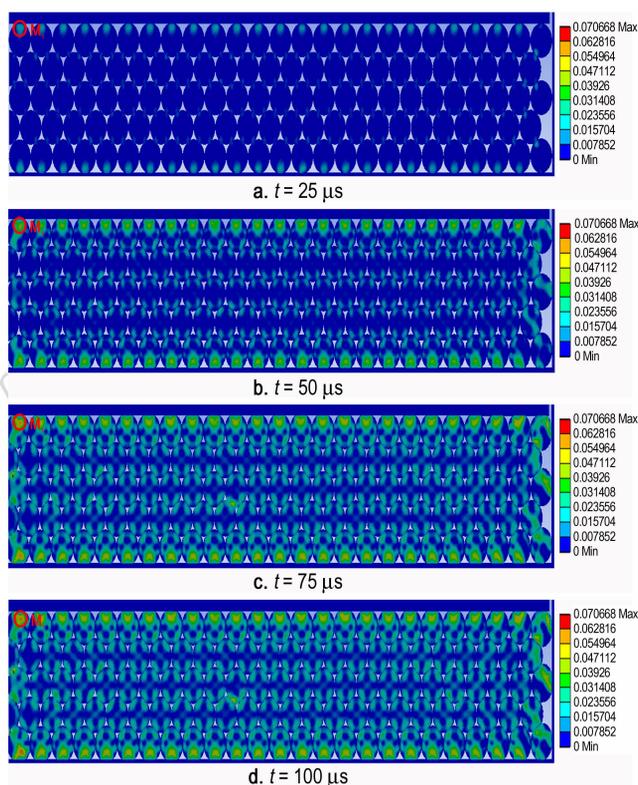


Fig. 8 Equivalent plastic strain of HMX particles at different times in case of regular arrangement

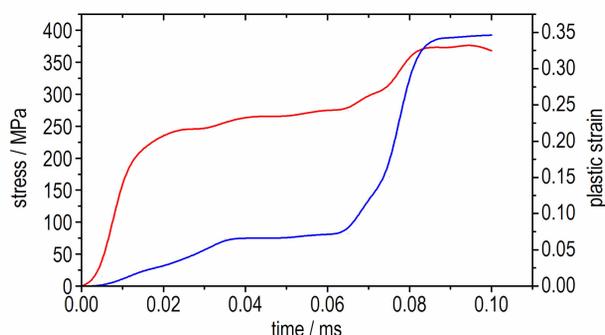


Fig. 9 Stress and plastic strain at M_1 point versus time curve in case of regular arrangement

Next, the account is taken into the case of irregular arrangement of particles. In the irregular arrangement, the HMX particles randomly packed. The arrangement includes 206 circular particles with diameters ranging from 40 mm to 300 mm. Fig. 10 and Fig. 11 show the calculated stress and plastic strain distributions in HMX particles with irregular arrangement at $t = 25 \mu\text{s}$, $t = 50 \mu\text{s}$, $t = 75 \mu\text{s}$ and $t = 100 \mu\text{s}$, respectively. Based on the simulation results, it is found that at point M_2 there is the maximum plastic work. Correspondingly, the curves of the stress and the plastic strain versus time at that point are shown in Fig. 12.

After the stress and plastic strain values of points M_1 and M_2 are obtained at different times, the temperature rise can be calculated by Eqs. (1) to (5). Table 3 presents the results of

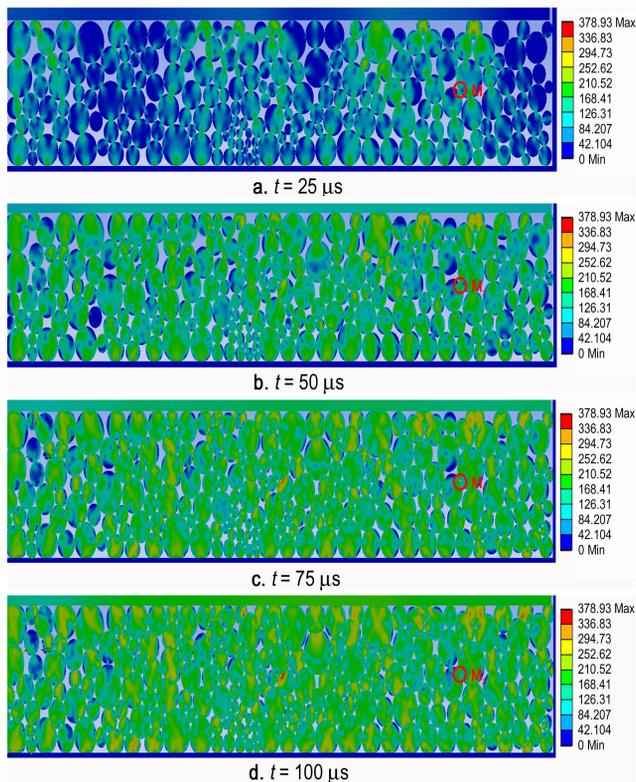


Fig. 10 Equivalent stress of HMX particles at different times in case of irregular arrangement

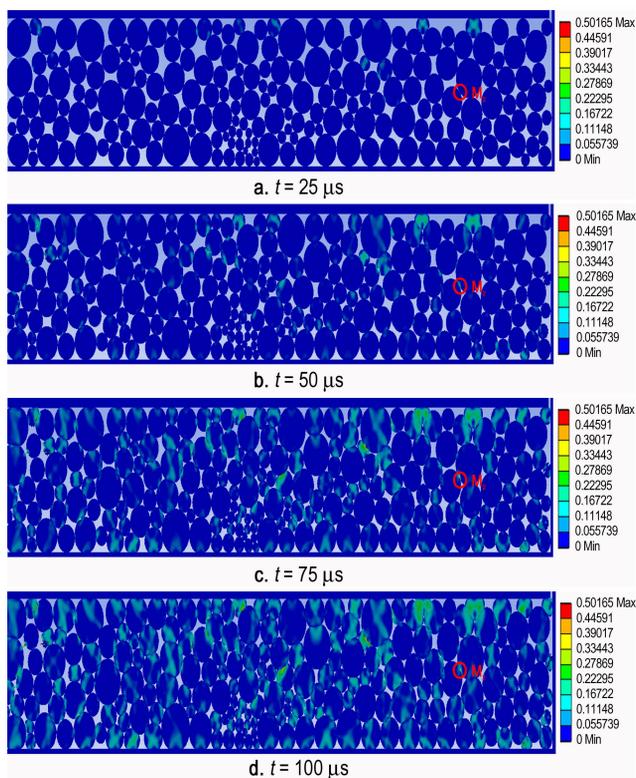


Fig. 11 Equivalent plastic strains in HMX particles at different times in case of irregular arrangement

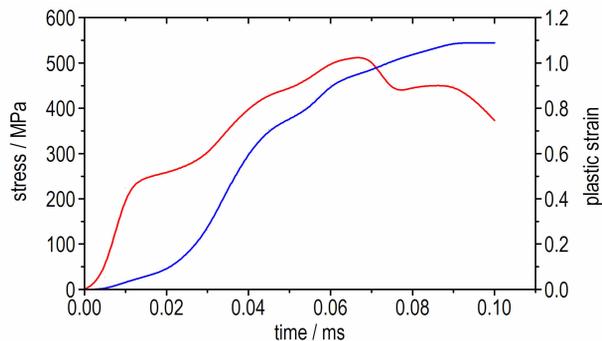


Fig. 12 Stress and plastic strain at point M_2 versus time in case of irregular arrangement

Table 3 Temperature rises at specific locations in two cases of HMX particle arrangement

point	M_1	M_2
$\Delta T/^\circ\text{C}$	37.2	142.9

the temperature rises obtained in this way. As it can be seen from the table, in the irregular arrangement of particles there gives great influence on HMX particle temperature rise, corresponding to the temperature rise of 142.9 °C. Rather, the temperature rise in the regular arrangement reaches 37.2 °C only. It indicates that the plastic work in the irregular arrangement of HMX particles has great contribution to the temperature rise. On the knowledge acquired from thermal test, the ignition temperature for HMX particles is 210 °C, so it is more reasonable in the simulation by considering the factor of irregular arrangement of the particles.

From the numerical simulations as well as calculations for temperature rise, it is found that the irregular arrangement of HMX particles can provide higher temperature rise in the particles than the regular arrangement. The difference comes from the sizes of the gaps between the particles. In the irregular arrangement, the particles with random distributions can form larger voids. The distribution of stress is uneven. In the larger gap area there is greater local plastic work.

3.3 Effect of Dropping Height on Temperature Rise in Irregular Arrangement

The difference of dropping height gives the different initial speed of the hammer. Higher dropping height passes a greater speed to the hammer. Owing that the irregular arrangement of particles produces much higher temperature rise in particles, we mainly focus our study on the case of irregular arrangement of particles. Let the hammer fall from different heights more than H_{50} , we calculate the temperature rises. To three kinds of the dropping heights of 40, 50 cm and 60 cm, the changes of

temperature rises at the location with maximum plastic work are calculated in the similar ways as given before. The obtained temperatures are presented in Table 4 for these situations.

As seeing from Fig. 13, the temperature rise in the particles increases with the rising of the height of the drop hammer. When the drop height reaches 60 cm, the temperature at point with maximum strain is 178.3 °C. This value is more closer to the ignition temperature of the HMX particles.

Table 4 Temperature rise values of HMX particles at different drop heights

H/cm	33	40	50	60
$\Delta T/^\circ\text{C}$	142.9	149.5	165.3	178.3

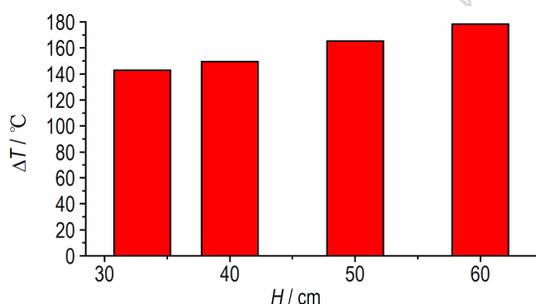


Fig. 13 Histogram of temperature rises with changes in drop heights

3.4 Effect of Reducing Yield Strength on Temperature Rise

In the above sections, we have calculated the temperature rises in the particles as the yield strength is selected to be 0.26 GPa. Now reducing the yield strength to 0.13 GPa, the calculation is operated and the temperature rise is calculated. The drop height is still H_{50} and the particles are packed in the form of the irregular arrangement. The purpose is to examine how the value of the yield strength affects the temperature rise in particles.

After simulations, the equivalent stress distribution and equivalent plastic strain distribution are shown in Fig. 14 and Fig. 15. As before, a point with maximum plastic work is designated with labelling by M_3 in the figures. In accordance to the temperature rise calculation by Eq. (1) to Eq. (5), the temperature rise at point M_3 is obtained to be 83.2 °C.

In the calculations, the changes of the yield strength value of the HMX particle material affect the temperature rise in particles greatly. When the yield strength is of smaller value, the temperature rise in particles is low. The explanation for this result is that under the same loading, as the yield strength is reduced, the stress values in particles are also reduced. Hence, the lower stresses lead to smaller plastic work while plastic strains vary in the same range. The temperature is naturally low from the smaller heat energy.

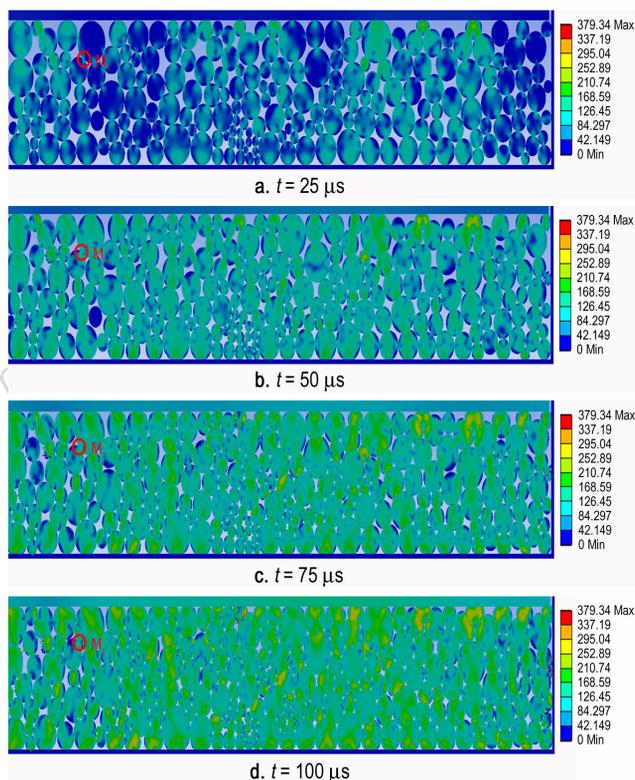


Fig. 14 Equivalent stresses of HMX particles at different times with 0.13 GPa yield strength

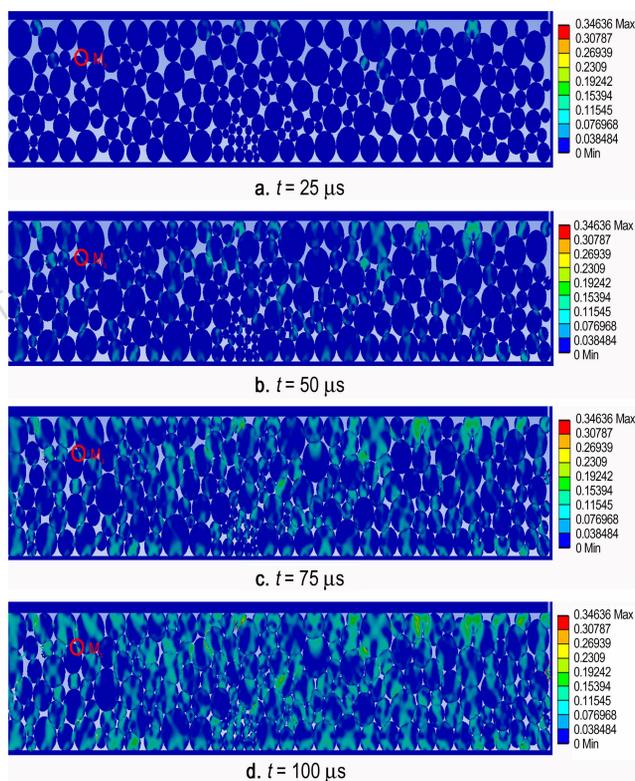


Fig. 15 Equivalent plastic strains of HMX particles at different times with 0.13 GPa yield strength

4 Conclusions

Through numerical simulation of drop hammer test for granular HMX, the local temperature rises of the particles can be calculated from the plastic deformation work of the particles. To experimental H_{50} critical drop height for HMX, and particles being under irregular arrangement, the maximum temperature rise in particles is calculated to be 142.9 °C. As the drop height is increased to 60 cm, the temperature rise reaches 178.3 °C. These predicted temperatures tend to initiate chemical reaction. However, also, the simulation does not provide the proof on the existence of the obvious inter-particle friction. On the influence of yield strength for explosive particles, smaller yield strength value leads to a lower temperature rise. The result indicates that the yield strength for explosive particles is one of the important factors in the prediction of temperature rise in drop hammer test.

At present, the chemical reaction and the self-heating process of particles are not included in the analysis. Even so, the obtained results on the temperature rises are tend to reach the ignition temperature of HMX explosive measured via ther-

mal analysis test. Regarding other factors that might cause the particle ignition will be studied in the future work.

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落锤试验撞击粒状 HMX 炸药变形及点火过程数值模拟

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摘要: 利用 AUTODYN 软件对落锤撞击粒状 HMX 炸药过程进行二维数值模拟。基于应力和塑性功的计算值, 通过塑性功转化热能的原理, 估算了颗粒中产生的温升。样品 HMX 颗粒为圆形几何形状, 假设颗粒具有弹塑性变形特性。颗粒堆放形式有规则排布和不规则排布两种情形。通过设定的落高和由自由落体公式计算出落锤的初始速度。针对落高分别为 33, 40, 50, 60 cm 的情况, 及样品颗粒材料不同屈服应力值(0.26, 0.13 GPa)进行计算, 得到落锤撞击颗粒时的温升变化。结果表明, 规则排布产生温度较低(37.2 °C), 而不规则排布产生温度较高(142.9 °C)。在不规则排布当中, 颗粒的局部塑性变形功可以导致较高的温升, 从而引起颗粒点火。同时考虑到 HMX 的屈服应力值的不确定性, 取较小屈服应力值(0.13 GPa)进行温升计算, 而其他计算条件相同, 得到的温升值仅为 83.2 °C, 比 0.26 GPa 时低 59.7 °C。

关键词: 落锤实验; HMX 颗粒; 数值模拟; 温升

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