

NUMERICAL STUDY OF THE FRICTIONAL INITIATION MECHANISM OF ENERGETIC MATERIALS UNDER LOW-VELOCITY IMPACT

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This paper presents the results of a comprehensive study on the frictional initiation mechanism of energetic materials (EM) under low-velocity impact. Based on data from physical experiments involving the penetration of a spherical impactor into an HMX-containing EM, a self-consistent mathematical model has been developed. This model describes the coupled motion of the impactor and the elastoplastic flow of the material. It accounts for the dissipation of the impactor's kinetic energy through plastic work and dry friction forces at the contact boundary, enabling the analysis of hot spot formation mechanisms. The Nelder–Mead algorithm was employed to solve the inverse problem, identifying key material strength parameters: yield strength and shear modulus. Numerical simulations of temperature fields were conducted for two loading regimes – with and without explosion initiation. The results of the computational experiment indicate that the conditions necessary for the onset of explosive transformation are achieved.

Keywords: friction heating; energy material; phlegmatized HMX; explosive transformation; strength parameters.

Introduction

Ensuring the safe storage and application of energetic materials (EM) is a critically important task, as their susceptibility to mechanical and thermal stimuli poses a potential risk of accidental initiation [1–3]. The primary dissipative processes responsible for the formation of hot spots in EM are friction (both external and internal) and the adiabatic compression of gas-filled cavities [4–6]. Investigating the initiation mechanisms of EM, including condensed-phase explosives, under mechanical stimuli is a relevant and complex challenge of critical importance for ensuring safety throughout the entire lifecycle of these substances. The relevance of this work stems from a fundamental contradiction: on one hand, modern trends in EM development aim to increase their energy density and performance, which inevitably leads to greater sensitivity to external stimuli; on the other hand, there are increasingly stringent safety requirements for the production, transportation, storage, and use of such materials, with the goal of completely preventing accidents under conditions of accidental mechanical or thermal loading.

Of particular complexity for prediction and modeling is the regime of low-velocity mechanical impact (less than 30 m/s), for which a single, universally accepted theoretical picture of initiation is still lacking [7–10]. In this context, the analysis of dissipative processes leading to the formation of local hot spots becomes key. Among these, frictional mechanisms are dominant, especially under conditions of shear deformation and contact interaction. These include both external friction at the boundary between the EM and inert materials or structural elements, and internal friction between particles and granules of the energetic composition itself.

Classical works that laid the foundation for the hot spot concept, along with subsequent research, have quantitatively defined initiation parameters for high-velocity impacts [4–6]. However, for low-velocity stimuli typical of many abnormal situations (drop, crush, friction), frictional heating [11, 12] can lead to the formation of a heated thin layer in the shear zone, which becomes a potential ignition source. Existing methods for assessing EM sensitivity [13–15] often lack universality precisely due to the diversity of possible initiation mechanisms, among which frictional initiation requires separate and detailed consideration.

Therefore, the aim of this work is a numerical study of the frictional initiation mechanism in energetic materials under low-velocity mechanical stimuli. The primary focus is on analyzing the conditions for the formation and evolution of heated layers at contact boundaries, as well as on discussing ways to apply this knowledge for developing improved hazard assessment methods and ensuring the safe handling of EM. The advancement of corresponding mathematical models for deformation and heat generation in thermoplastic materials will enable more accurate prediction of critical regimes and reduce the risks of uncontrolled ignition.

1. Experimental Data and Problem Statement

A series of physical experiments on low-velocity impact was presented in works [16]. The recorded parameters were the depth of the resulting indentation on the sample surface and the qualitative loading outcome: initiation of explosive transformation or its absence. Table 1 presents the data from a series of impact experiments on an HMX-containing energetic material. As noted in [16], the original methodology exhibited a phenomenon of the impactor rebounding and striking the sample surface again, which distorted the loading pattern. To obtain data for a single-impulse loading condition, a modified experiment (No. 6) was conducted with the following parameters: impactor mass of 2 kg, initial velocity of the spherical impactor 15.41 m/s.

Table 1

Data from the series of impact experiments on an HMX-containing energetic material

Experiment No.	Spherical Impactor Velocity, m/s	Penetration Depth, mm	Result
1	13.26	3.3	No explosion
2	27.5	4.83	Explosion
3	29.7	5.31	Explosion
4	26.9	5.40	Explosion
5	11.18	3.08	No explosion
6	15.41	3.15	No explosion

The schematic of the computational experiment corresponding to the physical setup is shown in Fig. 1. A spherical-nosed steel impactor with a cylindrical shank and a hemispherical tip of radius R_H moves with velocity \vec{V} ($V_r = 0$, $V_z = V$) and impacts the energetic material (EM) placed inside a rigid cylindrical casing. The mass of the impactor

is M . The objective is the mathematical modeling of the transient contact process to determine the stress, strain, and temperature fields in the EM.

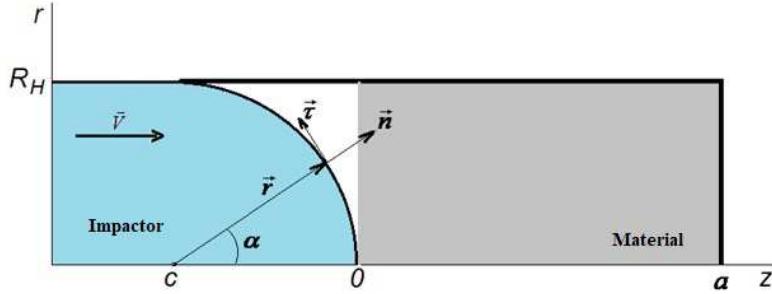


Fig. 1. Schematic of the impactor-EM interaction experiment.

2. Mathematical Model of Impactor Interaction with an Energetic Material

The mathematical model of the EM is based on the system of continuum mechanics differential equations describing transient elastoplastic flow. The equations are formulated in Lagrangian variables within a cylindrical coordinate system, which naturally accounts for the axisymmetric geometry of the problem, and take the following form:

$$\begin{aligned}
 \dot{\rho} &= -\rho \frac{\dot{V}}{V}, \quad \dot{V} = \nabla \cdot (v_{rr} + v_{\phi\phi} + v_{zz}); \\
 \rho \dot{v}_r &= \frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial S_{rz}}{\partial z} + \frac{S_{rr} - S_{\phi\phi}}{r}, \quad \rho \dot{v}_z = \frac{\partial \sigma_{zz}}{\partial z} + \frac{\partial S_{rz}}{\partial r} + \frac{S_{rz}}{r}; \\
 \rho \dot{U} &= -P \frac{\dot{V}}{V} + (S_{rr} v_{rr} + S_{\phi\phi} v_{\phi\phi} + S_{zz} v_{zz} + 2S_{rz} v_{rz}) - \nabla \cdot \mathbf{q}; \\
 \dot{S}_{rr}^0 &= 2\mu \left(v_{rr} - \frac{1}{3} \frac{\dot{V}}{V} \right); \quad \dot{S}_{zz}^0 = 2\mu \left(v_{zz} - \frac{1}{3} \frac{\dot{V}}{V} \right); \\
 \dot{S}_{\phi\phi}^0 &= -\dot{S}_{rr}^0 - \dot{S}_{zz}^0; \quad \dot{S}_{rz}^0 = 2\mu v_{rz}.
 \end{aligned} \tag{1}$$

Here ρ , v_i are the mass density and velocity, v_{ik} is the strain rate tensor, V is the volume, σ_{ik} is the non-equilibrium stress tensor, P , S_{ik} are the spherical part and deviator of the stress tensor, U is the specific internal energy per unit mass, T is the temperature, $\mathbf{q} = -\kappa \nabla T$ is the heat flux described by Fourier's law, and κ is the thermal conductivity coefficient. This system is closed with the material equations of state [17, 18] and boundary conditions that account for the interaction between the impactor and the material. To solve the system of equations (1), a numerical method for continuum mechanics equations, described in [19], was employed.

To describe plastic flow, the Prandtl–Reuss model [20, 21] was employed, in which the plastic strain rate tensor appears explicitly.

$$\dot{S}_{ik} = 2\mu (\hat{v}_{ik} - \dot{u}_{ik}^p), \tag{2}$$

where $\hat{v}_{ik} = v_{ik} - v_{ll}\delta_{ik}/3$, \dot{u}_{ik}^p is the plastic strain rate tensor, which is related to the stresses through the Mises flow rule $\dot{u}_{ik}^p = S_{ik}/\lambda$, λ is the plasticity modulus, and μ is the shear modulus. Equation (2) expresses the fundamental principle that elastic stresses are governed solely by elastic deformations.

The modulus of plasticity is found from the expression:

$$\frac{1}{\lambda} = \frac{3}{2} \frac{S_{ik}\hat{v}_{ik}}{Y_0^2}.$$

Combining the Mises criterion with (2) yields the equation for the deviatoric stress tensor:

$$\dot{S}_{ik} + \frac{S_{ik}}{\tau^p} = 2\mu\hat{v}_{ik},$$

where $\tau^p = \frac{\lambda}{2\mu}$ is the relaxation time of elastic stresses due to plastic flow (Maxwell relaxation time).

Work [16] provides a detailed description of the contact interaction model, encompassing the underlying physical processes, the mathematical formulation of boundary conditions incorporating friction forces, and an analysis of the sliding regime at the impactor–energetic material interface.

The model assumes that the impactor's deformation is negligible and that all its kinetic energy is dissipated through irreversible plastic deformation and changes in the thermodynamic state of the sample. Due to this interaction, the impactor's velocity decreases to zero, after which the elastic energy stored in the deformed material may cause its reverse motion (rebound).

Within this model framework, the impactor's motion is considered one-dimensional. It is subjected to an elastic resistive force from the material, which depends on the current contact area, as well as an additional force due to the work of dry friction forces at the contact boundary. Accounting for energy dissipation via friction is critical for accurately describing the impactor's deceleration.

Thus, the equation for the impactor velocity, accounting for the contribution of the friction force, can be written as follows:

$$V(t + \Delta t) = \sqrt{\left(V(t) + \frac{F_r}{M}\Delta t\right)^2 - \frac{4\pi}{M}\Delta t \int_0^{r_c} q_f r dr}, \quad (3)$$

where $F_r = 2\pi \int_0^{r_c} \Sigma_z(r) r dr$ is the force acting on the surface of the impactor embedded in the material, $\Sigma_z = \sigma_{zz}n_z + \sigma_{zr}n_r$ is the surface force, σ_{ik} are the components of the material stress tensor, $\mathbf{n}(n_r = \sin \alpha, n_z = \cos \alpha)$ is the normal vector to the impactor surface (Fig. 1), r_c is the coordinate of the contact boundary between the material and the impactor, and q_f is the heat flux generated by the work of dry friction forces.

Thus, to solve the stated problem of modeling the contact interaction between a spherical impactor and an EM under low-velocity impact, a self-consistent mathematical model was developed. The model describes the coupled motion of the rigid impactor and the deformable EM, treating them as a single mechanical system.

The equations of motion for the impactor and the constitutive relations for the EM, describing its elastoplastic behavior, are solved simultaneously. A key aspect of the model is the account of the kinetic energy dissipation of the impactor, which is expended on

plastic work and changes in the internal energy of the EM, as well as on overcoming friction forces at the contact interface. Consequently, the model establishes a quantitative link between the macroscopic motion of the impactor and the processes of deformation and energy release in the local contact region, providing a basis for analyzing the conditions for possible thermal initiation of the EM.

3. Determination of the Strength Characteristics of an Energetic Material

The numerical model of EM charge deformation under impact loading, implemented within a computational framework, is based on the Prandtl–Reuss elastoplastic model. The key parameters of this model are the elastoplastic material properties that define its strength and deformation characteristics, such as yield strength, shear modulus, and plastic flow conditions. Determining the elastic constants for EM is challenging due to the complex and heterogeneous microstructure of actual charges, which precludes the direct use of handbook data to describe their mechanical response. In this work, a combined approach was employed to calibrate the model, based on comparing numerical simulation results with experimental data on impactor penetration depths. The calibration method applied here extends the approach presented in [16]. Its key distinction and novelty lie in two aspects: 1) the development of a specialized computational algorithm for optimizing the set of strength parameters; 2) the use of experiment No. 6 as a benchmark, whose parameters minimize uncertainty and provide a reliable basis for model identification.

To proceed with the solution of the parameter identification problem, it is necessary to formally define the concept of the best fit between experimental data and numerical simulation results. In this work, a quantitative measure of this agreement is provided by an objective function (residual functional) $J(\boldsymbol{\alpha})$, which depends on the vector of unknown parameters $\boldsymbol{\alpha} = \{Y, \mu\}$.

The mathematical formulation of the problem is stated as a minimization task:

$$\hat{\boldsymbol{\alpha}} = \arg \min_{\boldsymbol{\alpha}} J(\boldsymbol{\alpha}).$$

The mean squared error (MSE) functional was chosen as the objective function, defined as follows:

$$J(\boldsymbol{\alpha}) = \frac{1}{N} \sum_{i=1}^N (Z_{\text{exp}}(t_i) - Z_{\text{calc}}(t_i, \boldsymbol{\alpha}))^2, \quad (4)$$

where $Z_{\text{exp}}(t_i)$ is the experimental value at time t , $Z_{\text{calc}}(t_i, \boldsymbol{\alpha})$ is the calculated value at time t obtained for a given parameter vector $\boldsymbol{\alpha}$, and N is the total number of experimental data points.

The minimization of the objective functional $J(\boldsymbol{\alpha})$ was performed using the Nelder–Mead algorithm [22], which combines simplicity of implementation, no requirement for gradient information, and high efficiency for low-dimensional problems.

The minimization of the mean squared error (4) was performed via numerical simulations with different sets of strength parameters for the studied EM. The resulting penetration depth was then compared with experimental data, and the MSE was computed. If the error exceeded a predefined threshold, a new parameter set was generated using the Nelder–Mead algorithm, and the simulation–comparison–evaluation

cycle was repeated. Iterations continued until a convergence criterion was met, ensuring an acceptable agreement between the model and the experiment.

The values obtained from the optimization procedure for different initial guesses converged to the same parameter set. This confirms that the global minimum of the objective function corresponds to the strength parameter values of $Y = 58.94$ MPa, $\mu = 39.49$ GPa

The penetration depth profile of the spherical impactor obtained with the identified parameter set is presented in Fig. 2.

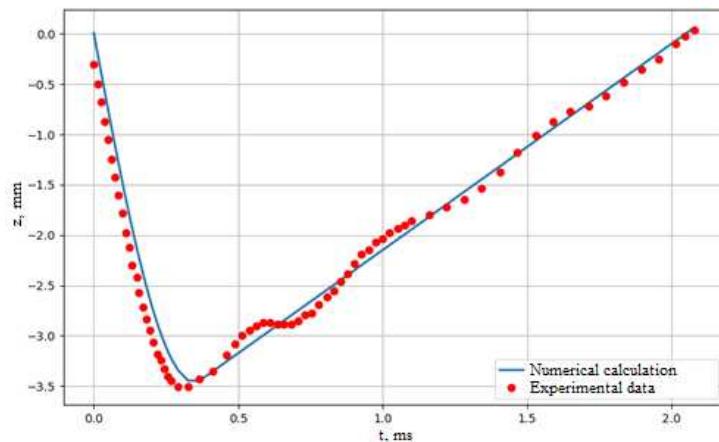


Fig. 2. Comparison of the numerical simulation with the experiment for the parameter set $Y = 58.94$ MPa, $\mu = 39.49$ GPa

4. Results of Numerical Simulation

A potential mechanism for initiating explosive transformation under low-velocity impact by a spherical impactor is the intensive local heating of the EM in the contact zone. The primary sources of heat generation in the considered model are [9]:

1) Dissipation of mechanical energy during bulk deformation – the work expended on plastic deformation of the material is almost entirely converted into heat in accordance with the adopted hypothesis of adiabatic heating.

2) Heat generation at the contact surface – the work performed by dry friction forces at the impactor-EM interface, the power of which is determined by the sliding conditions and the normal stress. The combined action of these two factors leads to the formation of hot spots in the near-contact region, which can serve as a cause for the thermal ignition of the exothermic reaction in the EM.

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This section presents a comparative analysis of numerical simulation results for temperature field formation in the EM for Experiments No. 3 and No. 6. These experiments represent two fundamentally different response scenarios to low-velocity impact: Experiment No. 3 resulted in the initiation of an explosive transformation, while initiation did not occur in Experiment No. 6. The figures below visualize:

1. The temperature distribution within the EM volume up to the boundary with the thin near-surface layer.

2. The temperature profile directly at the contact interface within this thin layer, where maximum gradients and frictional heating are realized.

This analysis makes it possible to evaluate the contributions of bulk plastic deformation and contact friction to the overall thermal balance and to identify critical regions with temperatures potentially sufficient for initiation.

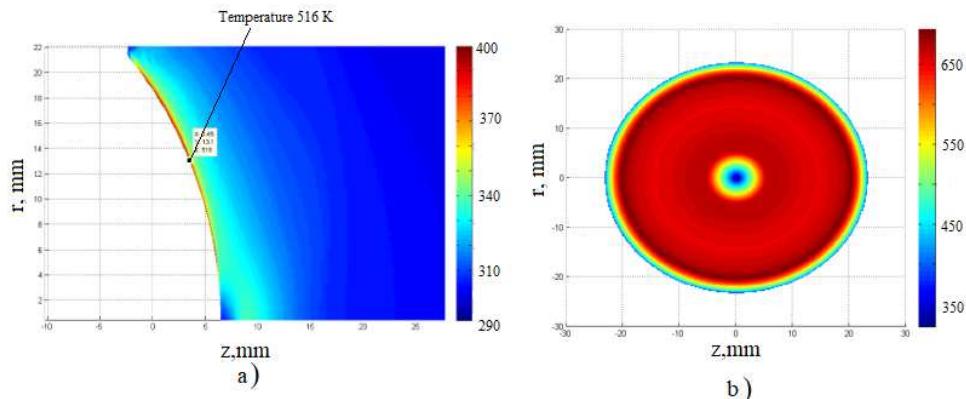


Fig. 3. Numerical results for Experiment No. 3: (a) temperature field within the EM volume; (b) temperature distribution at the contact interface in the thin surface layer

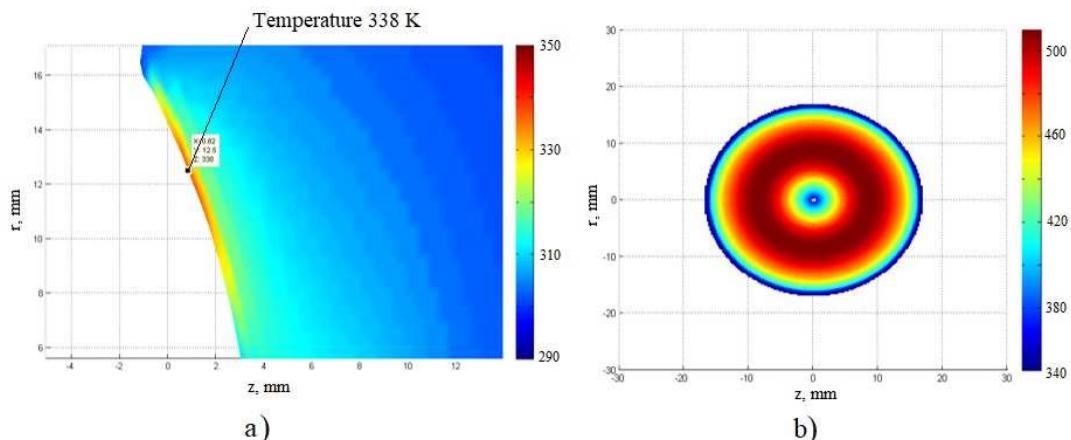


Fig. 4. Numerical results for Experiment No. 6: (a) temperature field within the EM volume; (b) temperature distribution at the contact interface in the thin surface layer

A qualitative comparison was performed between the results of the present numerical modeling and those reported in [9], which investigated the impact of spherical impactors (mass 2–100 g) on phlegmatized HMX. Despite differences in the material composition and scale of the experiments, a fundamental correspondence is observed in the contact pattern. The authors of [9] reported the formation of two characteristic zones on the impactor surface: a central region (45° – 54°) without wear marks and a surrounding annular region (100° – 114°) with signs of abrasive action, which was identified as a potential reaction site.

Within the framework of the present model, a similar annular zone of maximum frictional heating (87.05° – 97.58°) is predicted for all considered experiments, while the central zone (0° – 43.48° – 55.61°) exhibits negligible heating, driven solely by bulk plastic

deformation. Thus, the numerical simulation results are consistent with the experimental observations in [9] regarding the spatial localization of the intensive contact interaction zone responsible for potential initiation.

The numerical simulation results demonstrate that conditions for the formation of a local hot spot are established at the “energetic material – spherical impactor” contact interface, primarily due to energy dissipation by friction forces. For a quantitative assessment of the material’s thermal stability in this region, it is appropriate to estimate the adiabatic induction period preceding the onset of a self-accelerating reaction. For this purpose, a relation widely used in thermal explosion theory is employed [11, 23]:

$$t_{ad} = \frac{\rho c_p}{Q z_0} \frac{RT^2}{E_a} \exp \left(\frac{E_a}{RT} \right), \quad (5)$$

where c_p is the specific heat capacity at constant pressure, Q is the heat of reaction (5526 kJ/kg [24]), z_0 is the pre-exponential factor ($5 \times 10^8 \text{ s}^{-1}$ [24, 25]), R is the universal gas constant ($8.314 \text{ J}/(\text{mol}\cdot\text{K})$), T is the temperature (K), and E_a is the activation energy (219.300 J/mol [24]). The specific heat capacity of HMX is determined from its temperature dependence given in [25] for different temperature ranges. The profiles of the maximum temperature achieved in the thin EM layer during the numerical simulations of Experiments No. 3 and No. 6 are presented in Figs. 5 and 6 below.

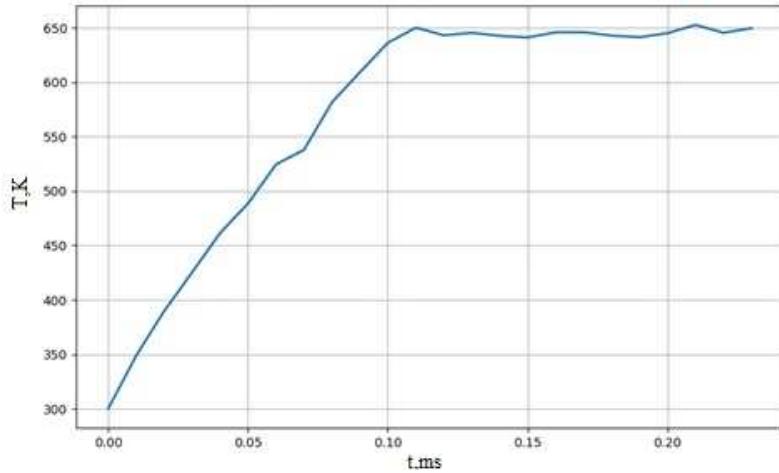


Fig. 5. Time dependence of the maximum temperature in the thin EM layer for Experiment No. 3

According to the simulation results, active melting in the sample begins at a temperature of 650 K. Although the melting point of HMX at atmospheric pressure is 552 K [24, 25], under the conditions of high confining pressure characteristic of contact loading, a significant shift of the phase transition line to higher temperatures occurs [12], making the obtained value physically plausible.

For the characteristic temperature level of 635 K in the hot spot region, the adiabatic induction period was calculated to be 0.11 ms. This time is shorter than the duration of the impactor’s contact interaction (Fig.5), which, according to the model, allows the thermal induction process to be completed before the mechanical loading ceases. This finding, supported by the observed development of the high-temperature zone, unequivocally

indicates the possibility of initiating explosive transformation under these conditions, which is consistent with the results of physical experiments.

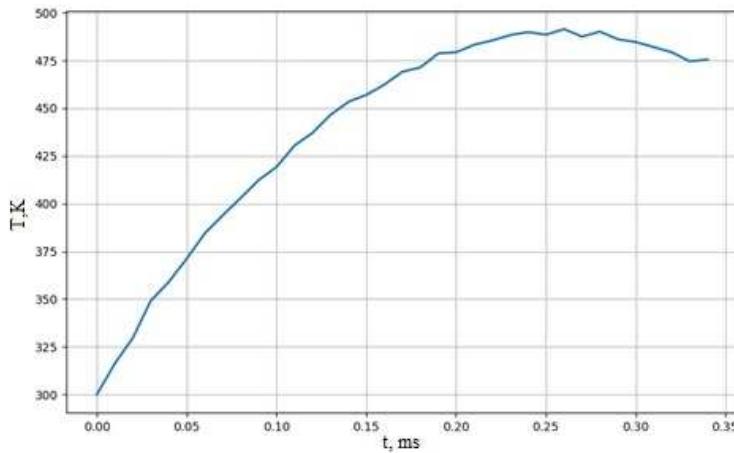


Fig. 6. Time dependence of the maximum temperature in the thin EM layer for Experiment No. 6

The temperature profile at the contact surface over time (Fig. 6) shows that its maximum value does not reach the material's melting threshold when accounting for the latter's increase under pressure. This indicates that the rate of mechanical energy dissipation (the combined contribution of friction and plastic work) was insufficient to generate a thermal impulse capable of overcoming the heat loss barrier. Consequently, in this experiment, the impactor's kinetic energy was either dissipated within the volume in a time shorter than the characteristic thermal induction time, or the energy release density in the contact zone did not reach the critical level required for initiation. This conclusion is consistent with the results of the physical experiments.

5. Conclusion

Based on a comprehensive study integrating numerical modeling and physical experiments, the initiation mechanism of EM under low-velocity impact has been identified as intensive frictional heating in the contact interaction zone. This enables the formulation of the following science-based recommendations for targeted reduction of EM impact sensitivity:

1. To reduce the heat generation rate in the contact region, a targeted modification of the EM formulation is recommended. The introduction of phlegmatizing agents or solid lubricant additives that lower the friction coefficient at interparticle and external boundaries is an effective way to suppress hot spot formation.

2. The developed mathematical model, implemented as a software package, enables the identification of critical zones of thermal risk through the analysis of calculated temperature fields and their correlation with initiation/no-initiation outcomes. This tool should be applied to optimize contact interfaces and operational regimes to eliminate local overheating exceeding the material's thermal decomposition threshold.

An algorithm for solving the inverse optimization problem was developed, allowing for the determination of key EM strength parameters – yield strength and shear modulus. The identified set of material characteristics can be used for further modeling and analysis of other initiation mechanisms, such as energy dissipation through internal friction or

adiabatic compression of gas inclusions, relevant for both low- and high-velocity loading regimes.

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ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ ФРИКЦИОННОГО МЕХАНИЗМА ИНИЦИРОВАНИЯ ЭНЕРГЕТИЧЕСКИХ МАТЕРИАЛОВ ПРИ НИЗКОСКОРОСТНОМ УДАРЕ

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В статье представлены результаты комплексного исследования фрикционного механизма инициирования энергетических материалов (ЭМ) при низкоскоростном ударе. На основе данных натурных экспериментов по внедрению сферического ударника в октогенсодержащий ЭМ разработана самосогласованная математическая модель, описывающая сопряжённое движение ударника и упругопластическое течение материала. Модель учитывает диссиацию кинетической энергии ударника за счёт пластической работы и сил сухого трения на контактной границе, что позволяет анализировать механизм образования горячих точек. С использованием алгоритма Нелдера–Мида для решения обратной задачи найдены прочностные параметры материала: предел текучести и модуль сдвига. Проведено численное моделирование температурных полей для двух режимов нагружения – с инициированием взрыва и без него. Результаты вычислительного эксперимента указывают на достижение условий, необходимых для начала взрывного превращения.

Ключевые слова: фрикционный разогрев; энергетический материал; флегматизированный октоген; взрывчатое превращение; прочностные параметры.

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