

# Modeling of PETN Initiation by an Electron Pulse with Nanosecond Duration

A.V. Khanefit and E.V. Duginov

Kemerovo State University, 6, Krasnaya, Kemerovo, 650043, Russia  
E-mail: khanefit@kemsu.ru

**Abstract** – Numerical modeling of PETN initiation has been carried out by an electron pulse. A system of the equations of unbound thermoelasticity has been solved. An implicit difference circuit was used. Experimental distribution of absorbed energy density of an electron beam was approximated by a third degree polynomial. Phase transition (PETN fusion) and the dependence of activation energy of an exothermic reaction from mechanical pressure were taken into account. Distributions of temperature, pressure, deformation, displacement of particles, and the dynamics of an acoustic pulse of compression – stretching were calculated.

## 1. Introduction

Over the last few years physical and chemical processes in PETN under the impact of electron pulses with nanosecond duration have been intensively studied. The thresholds of mechanical destruction and the critical density of the electron beam energy  $W^*$ , resulting in the PETN ( $W^* \sim 15 \text{ J/cm}^2$ ) initiation [1–5] have been determined. There are two points of view on the mechanism of PETN initiation with an electron pulse: electric breakdown [3] and thermal explosion [4]. The critical energy density of PETN initiation by a laser pulse with the diameter of the beam more than 1 mm, is about  $15 \text{ J/cm}^2$  [6]. It suggests that PETN initiation by laser and electron pulses could occur by means of one and the same mechanism, viz. thermal.

When an electron beam is absorbed by the condensed explosive, thermoelastic stresses in solid state arise in addition to heating. Elastic stresses can change activation energy of a solid state chemical reaction [7]. It results in a feedback in the system: an exothermic reaction – elastic mechanical stresses. It can be both positive, and negative, that is, it can both reduce the explosive initiation threshold, and increase it.

## 2. Mathematical model

To study the given problem, the numerical solution of a one-dimensional nonlinear equation of heat conductivity has been carried out:

$$c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} + \frac{\Lambda(x)}{R_e} I(t) + qK_0 \exp\left(-\frac{E}{k_B T}\right) \quad (1)$$

together with a wave equation for thermoelastic stresses

$$c_s^2 \frac{\partial^2 \sigma}{\partial x^2} - \frac{\partial^2 \sigma}{\partial t^2} = 3\alpha_l K \frac{\partial^2 T}{\partial t^2}. \quad (2)$$

Equations (1) and (2) have the following initial and boundary conditions:

$$T(x, 0) = T_0, \quad -\lambda \left. \frac{\partial T}{\partial x} \right|_{x=0} = -j_s L, \quad \left. \frac{\partial T}{\partial x} \right|_{x=h} = 0, \quad (3)$$

$$\sigma(0, x) = 0, \quad \left. \frac{\partial \sigma}{\partial t} \right|_{t=0} = 0, \quad \sigma(t, 0) = -p, \quad \sigma(t, h) = 0. \quad (4)$$

Here  $h$  is the sample thickness;  $T$  is the temperature;  $\lambda$ ,  $c$  are the coefficient of heat conductivity and heat capacity of the material;  $\rho$  is the density of matter;  $q$ ,  $K_0$ ,  $E$  are the heat effect of reaction, pre-exponential factor of the decomposition reaction, activation energy of the decomposition rate, respectively;  $j_s$  is the flow of particles evaporating from the surface;  $L$  is the heat of evaporation;  $k_B$  is the Boltzmann constant;  $R_e$  is the electron free effective path length;  $I(t)$  is the energy flux density of electron beam;  $\Lambda(x)$  are the absorbed energy distribution of electron beam;  $c_s$  is the adiabatic velocity of sound;  $\sigma$  is the stresses along of surface normal;  $K$  is the modulus of dilatation;  $\alpha_l$  is the coefficient of linear thermal expansion.

The time dependence of the electron pulse intensity was specified as

$$I(t) = \frac{W}{6\tau_m} \left( \frac{4t}{\tau_m} \right)^4 \exp\left(-\frac{4t}{\tau_m}\right),$$

where  $\tau_m$  is the duration of the first front of the pulse concerning the pulse duration, measured on the half-height by the expression  $\tau_i = 1.19\tau_m$ ;  $W$  is the energy density of the electron pulse.

Experimental distribution of density of the absorbed energy of an electron pulse [4] was approximated by the third degree polynomial

$$\Lambda(\xi) = 0.7 + 1.57\xi - 2.31\xi^2 + 0.61\xi^3, \quad (5)$$

where  $\xi = x/R_e$  ( $R_e = 173.6 \cdot 10^{-4} \text{ cm}$ ). Equation (5) has a maximum:  $\Lambda_m = \Lambda(\xi_m) = 1$  at  $\xi_m = 0.405$ . In addition, it is assumed that the function  $\Lambda(\xi) = 0$  at  $\xi \geq 1.44$  and the integral

$$\int_0^{1.44} \Lambda(\xi) d\xi = 1.$$

Dependence of activation energy of an exothermic reaction was taken as the linear function from elastic stresses [7]

$$E(x) = E_a + \sigma(x, t) \Delta V^\ddagger, \quad (6)$$

where  $E_a$  is the activation energy of the decomposition rate PETN at  $\sigma = 0$ ;  $\sigma \Delta V^\ddagger$  is the physical activity brought about by elastic stresses during the reaction;  $\Delta V^\ddagger$  is the activation volume. Activation volume is equal to the difference in the volume of the activated complex and that of the reagents at the start state [7]. Depending on the character of  $\sigma$  and  $\Delta V^\ddagger$  it is possible both to increase the activation energy of thermal decomposition of PETN and to reduce it. Thus, in the system of equations (1), (2) there is a feedback which can be both positive and negative.

Dynamic pressure of PETN evaporating molecules was calculated in terms of the formula

$$p = m u_s j_s.$$

Here,  $m$  is the PETN molecule weight;  $u_s$  is the velocity of PETN molecules evaporating from the surface of a solid, determined by expression [8]

$$u_s = \sqrt{\frac{k_B T_s}{2\pi m}},$$

where  $T_s$  is the surface temperature of PETN.

Besides a pressure in work have calculated deformation of solid body

$$\varepsilon = \frac{1}{\rho c_0^2} [\sigma + 3\alpha_r K (T - T_0)] \quad (7)$$

and moving of particles of the condensed matter

$$u(x) = \int_0^x \varepsilon(x) dx. \quad (8)$$

The expression for the density at the beam of PETN evaporating molecules was solved as

$$j_s = j_0 \exp\left(-\frac{L}{k_B T}\right),$$

where  $j_0 = 10^{32} \text{ m}^{-2} \cdot \text{s}^{-1}$  is the preexponent of density at the beam.

The numerical solution of a one-dimensional equation of heat conductivity with nonlinear sources of heat (1) and initial and boundary conditions (3) was carried out using of the conservative implicit circuit. To solve a wave equation for thermoelasticity (2) with initial and boundary conditions (4), a half implicit circuit of the second order of accuracy was used. The received system of difference equations was solved by the chaser method. The difference net was homogeneous both on coordinate and on time.

PETN fusion was taken into account at numerical realization of the algorithm to solve the equation of

heat conductivity. Phase transition was taken into account as follows. When,  $T_f$  is achieved in any "i" layer of the difference net on coordinate, the temperature in this area stops changing and the process of fusion begins. Since this moment, the process of fusion occurs by means of the energy liberated at absorption of an electron beam, the energy liberated during an exothermic reaction, and the energy consumed on heat conductivity:

$$\Delta Q_i = c \rho \Delta T_i = \Delta t \left[ \lambda \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} + \frac{\Lambda(x_i)}{R_c} I(t) + q K_0 \exp\left(-\frac{E_f}{k T_i}\right) \right], \quad (9)$$

where  $\Delta t$  and  $\Delta x$  are steps on time and coordinate accordingly. As soon as the accumulated energy in a layer becomes equal to the product

$$\sum \Delta Q_i = \rho H_f,$$

where  $H_f$  is the latent heat of fusion, the temperature of a layer starts changing again.

The calculations were carried out with  $T_0 = 300 \text{ K}$  and the following thermo-physical and kinetic parameters of an PETN:  $c = 1.255 \cdot 10^3 \text{ J/(kg} \cdot \text{K)}$ ,  $\lambda = 0.1004 \text{ W/(m} \cdot \text{K)}$ ,  $\rho = 1.77 \cdot 10^3 \text{ kg/m}^3$ ,  $q = 4.184 \cdot 10^9 \text{ J/m}^3$ ,  $K_0 = 10^{16} \text{ s}^{-1}$ ,  $E_a = 1.717 \text{ eV}$  [9],  $c_s = 2320 \text{ m/s}$ ,  $\alpha_r = 0.773 \cdot 10^{-4} \text{ K}^{-1}$ ,  $K = \rho c_s^2 = 9.52 \cdot 10^9 \text{ Pa}$  [10],  $L = 1.0 \text{ eV}$  [11],  $T_f = 413 \text{ K}$ ,  $H_f = 192 \text{ kJ/kg}$  [12].

We neglected the difference between thermo-physical and kinetic parameters of the melt and a PETN single crystal as it is not known how the given parameters can change.

Activation volume of  $\Delta V^\ddagger$  varied from  $+3 \cdot 10^{-10}$  up to  $-3 \cdot 10^{-10} \text{ eV/Pa}$ .

### 3. Results and discussion

We make calculations at different electron pulse durations and energy densities. Thickness  $h$  of a PETN crystal varied from 1 up to 1.5 mm. The results of the numerical solution to the problem of condensed material ignition are submitted in Figs. 1–4.

Dynamics of temperature change of PETN  $\Delta T$  ( $\Delta T = T - 300 \text{ K}$ ) in the field of absorption of an electronic beam at energy density of an electronic pulse exceeding critical energy  $W = 20 \text{ J/cm}^2$ ,  $\tau_i = 15 \text{ ns}$  is presented in Fig. 1. As seen, gradation caused by fusion of a crystal appear on the curves of temperature distribution  $\Delta T$  (curves 2, 3).

Calculations of time of delay of PETN initiation by an electron pulse depending on activation volume of  $\Delta V^\ddagger$  at various sizes of a crystal are submitted in Fig. 2. Time of delay was determined from the condition, that

$$\left. \frac{d\Delta T_m}{dt} \right|_{t=t^*} \rightarrow \infty.$$

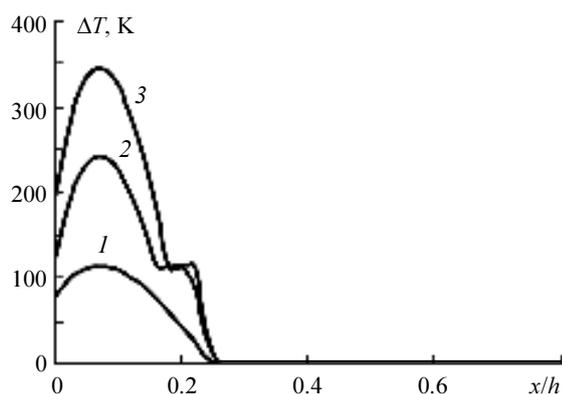


Fig. 1. Temperature distribution  $\Delta T$  in a sample absorbing an electron beam at various time instants:  $t = 1 \cdot 10^{-8}$  (1),  $2 \cdot 10^{-8}$  (2),  $3 \cdot 10^{-8}$  s (3)

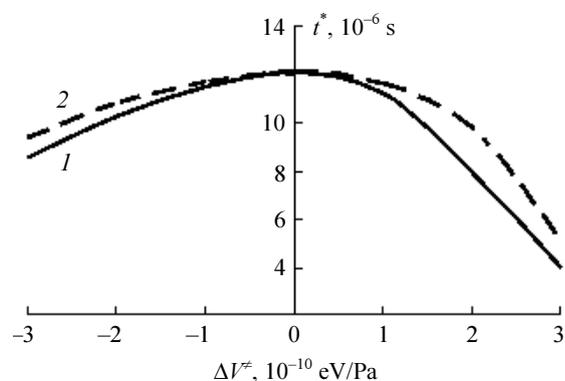


Fig. 2. Influence of activation volume  $\Delta V^*$  on the time of delay of PETN initiation by electronic pulse at  $W = 20$  J/cm<sup>2</sup>,  $\tau_p = 15$  ns:  $h = 1$  (1); 1.5 mm (2)

From Fig. 2 it is seen that the curves  $t^* = f(\Delta V^*)$  have their maximum at  $\Delta V^* = 0$ , not depending on crystal thickness. Time of delay, not depending on the character of the activation volume, and, hence threshold density of electron pulse energy of PETN initiation with  $\Delta V^*$  increase in modulo, decrease. It is explained by the fact that thermoelastic stresses which move along the crystal as waves, arise (Fig. 3) at absorption of energy of an electron beam and further self-heating of PETN by means of an exothermic reaction.

From Fig. 3 it is seen that at the beginning there is a generation of waves of compression ( $\sigma < 0$ ), passing, in due course, into waves of stretching ( $\sigma > 0$ ). Recurrence of the given process occurs periodically. Thus, waves of elasticity at pulse impact, independent of the character on activation volume, stimulate the PETN initiation. Time of delay of initiation depends on crystal thickness. Experimental detection of the effect would prove the dependence of activation energy of a chemical reaction from a mechanical stress.

From Fig. 3 it is also seen that sort of "two" running waves of elasticity appear in a crystal. The given effect is connected to the fusion process of PETN in the field of irradiation. The first wave is generated before the moment of fusion, and the second one,

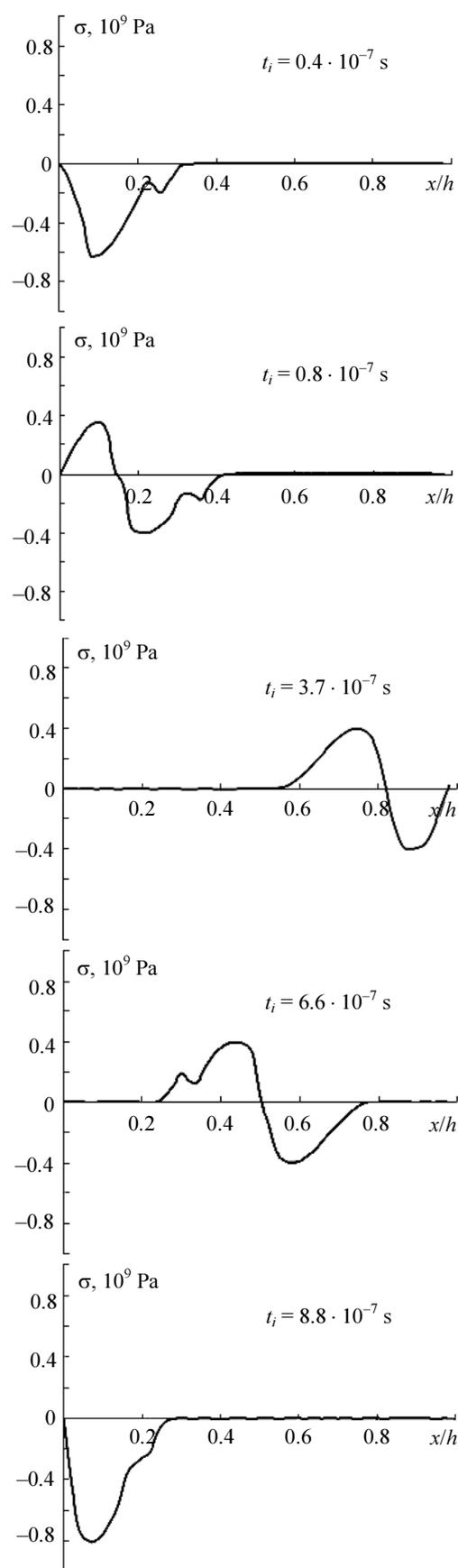


Fig. 3. Dynamics of distribution of thermoelastic waves of pressure in the volume of a crystal

some time after the moment of fusion. It results in the appearance of the “shelf” on the curve of pressure distribution dependence in the volume of a crystal ( $t = 0.2 \cdot 10^{-7}$  s) which in due course is deformed.

Arising stretching pressures can cause breaks inside a solid. Cutting destruction of a sample in section  $x$  can take place when the maximum value of stretching pressure in this section is equal to dynamic tensile strength durability of a substance. It is necessary to note that elastic mechanical pressures arising in PETN are commensurable with its strength limit and explosion by impact [13]. However, we do not discuss this problem here because a thermoelastic stress depends on the module of uniform compression and the factor of linear expansion. These parameters for the PETN melt are unknown. Though, preliminary calculations have shown that linear expansion factor increase in the given model results in initiation threshold decrease.

Calculations of displacement of a back surface of a sample are presented in Fig. 4.

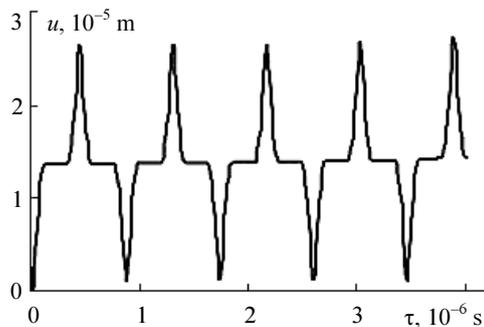


Fig. 4. Dynamics of displacement of a back surface of a sample

The calculations were carried out by numerical integration of expression (8) substituting the top limit  $x$  by  $h$ . From Fig. 4 it is seen, that the displacement of a back surface of a sample is of oscillatory character. These oscillations are periodic. The period of oscillation (a period of time between two nearest maxima)  $\tau \approx 860$  ns and determined by expression

$$\tau = 2h/c_s .$$

The fluctuations generate an acoustic signal. Frequency of acoustic vibrations  $\nu = c_s/2h \approx 1.16$  MHz.

The amplitude of acoustic vibrations increases with temperature increase. Period of acoustic vibrations vs. crystal size results in dimensional effect, i.e., the dependence of time of delay of initiation on crystal thickness. It can be accounted for by the fact that the

more the size of a crystal is, the longer waves of thermoelastic stresses are outside the zone of an exothermal reaction.

#### 4. Conclusions

1. PETN initiation by an electron pulse can be accounted for by the thermal mechanism.

2. The dimensional effect, i.e., the dependence of time of delay of initiation on crystal thickness, is found out.

3. At pulse non-uniform heating mechanical pressures reduce initiation threshold independent of the character of activation volume  $\Delta V^\#$ .

#### References

- [1] V.I. Korepanov, V.M. Lisitsyn, V.I. Oleshko, and V.P. Tsypilev, *Pis'ma Zh. Tekh. Fiz.* **29/16**, 23 (2003).
- [2] B.P. Aduiev, G.M. Belokurov, and S.S. Grechin, *Pis'ma Zh. Tekh. Fiz.* **30/15**, 91 (2004).
- [3] V.I. Oleshko, V.I. Korepanov, V.M. Lisitsyn, and V.P. Tsypilev, *Izv. Vyssh. Uchebn. Zaved. Fiz.* **10**, 204 (2006).
- [4] B.P. Aduiev, G.M. Belokurov, S.S. Grechin, and V.N. Shvaiko, *Izv. Vyssh. Uchebn. Zaved. Fiz.* **2**, 3 (2007).
- [5] V.I. Oleshko, V.I. Korepanov, V.M. Lisitsyn, and V.P. Tsypilev, *Fiz. Goreniya Vzryva* **43**, 87 (2007).
- [6] I.V. Tarzhanov, A.D. Zinchenko, V.I. Sdobnov, and B.B. Tokarev, *Fiz. Goreniya Vzryva* **32**, 113 (1996).
- [7] I.I. Aliev, A.L. Kovarskii, and A.L. Buchachenko, *Khim. Fiz.* **26/5**, 11 (2007).
- [8] S.I. Anisimov, Ya.A. Imas, G.S. Romanov, and Yu.V. Khod'ko, *Deistvie izlucheniya bol'shoi moschnosti na metally*, Moscow, Nauka, 1970, 272 pp.
- [9] A.F. Belyaev, V.K. Bobolev, A.I. Korotkov, A.A. Sulimov, and S.V. Chuiko, *Perexod goreniya kondensirovannykh sistem vo vzryv*, Moscow, Nauka, 1973, 293 pp.
- [10] A.A. Borisova, *Detonation and explosives*, Moscow, Mir, 1981, 392 pp.
- [11] F.A. Baum, K.P. Stanyukovich, and B.I. Shekhter, *Fizika vzryva*, Moscow, Nauka, 1959, 800 pp.
- [12] F.A. Baum, A. S. Derzhavec, and N.N. Sanasaryan, *Termoistoikie vzryvchatye veschestva i ikh deistvie v glubokikh skvazhinakh*, Moscow, Nedra, 1969, 160 pp.
- [13] G.T. Afanas'ev and V.K. Bobolev, *Initsirovanie tverdykh vzryvchatykh veschestv udarom*, Moscow, Nauka, 1968, 174 pp.