

Influence of absorbed energy distribution along beam radius on ignition threshold of condensed explosives

A V Khanef^{1,2}, G A Ivanov¹ and E V Duginov³

¹Kemerovo State University, Krasnaya, 6, Kemerovo, Russia

²National Research Tomsk Polytechnic University, 30, Lenin Avenue, Tomsk, Russia

³Kemerovo State Agricultural Institute, Markovtseva, 5, Kemerovo, Russia

E-mail: avkhanef@mail.ru

Abstract. The criterion of the condensed explosive ignition by the electron beam, which takes into account Gaussian distribution of electron density along the beam radius, has been obtained. It has been shown that radial heat removal of the absorbed energy leads to the increase in critical ignition energy if the effective track length of electrons in a solid is commensurate with the beam radius. The critical energy of PETN initiation by the electron beam has been calculated.

1. Introduction

The criterion of condensed explosive ignition by the short-duration electron beam was determined in the article [1]. The criterion was obtained on conditions that the rate of the chemical reaction on the border of the reaction layer is e times as small as the rate of the chemical reaction at the maximum of electron beam absorption, and the heat gain rate as a result of the chemical reaction in the solid Q_+ is to exceed the rate of heat removal from the reaction layer deep into the solid Q_- [2]. The obtained criterion didn't take into account the influence of the electron beam radius on the ignition threshold and the melting of the explosives. The track length of the explosives in the solid is known to depend on the initial kinetic energy of electrons. So, to estimate the critical energy of explosive ignition by the electron beam it is necessary to know at what electron energy the track length of electrons is commensurate with the beam radius as in this case radial heat removal from the absorption area needs to be taken into consideration [3]. The object of the current paper is to obtain the criterion of explosive ignition by the electron beam, which would take account of the melting of explosives and the beam radius, and the estimation of kinetic energy of electrons for PETN ($C_5H_8N_4O_{12}$) when the effective length of electrons is commensurate with the beam radius.

2. Problem statement

Let us analyze the following model. We consider the short-duration pulsed electron beam to fall normally on the surface of the solid parallel to axis z . As the short duration of the pulse we understand the duration when the diffusion of the heat from the area of electron absorption in the solid during the pulse duration can be neglected. We also assume the distribution of intensiveness along the beam cross-section to have Gauss shape [4]. In this case the temperature distribution along the crystal at the pulse decay is to be defined by the distribution of the absorbed energy:



$$T(\xi, r) = T_0 + \frac{W}{c\rho R_{ef}} \Lambda(\xi) \exp\left(-\frac{r^2}{r_0^2}\right), \quad (1)$$

where T_0 , T – the initial and current temperatures of the sample; W – the density of absorbed energy of the electron beam; r – the distance from the beam axis; r_0 – the beam radius; c , ρ – the heat capacity and the density of the sample; R_{ef} – the effective track length of the electrons; $\Lambda(\xi)$ – the distribution of the density of the absorbed beam energy along the thickness of the crystal; $\xi = z / R_{ef}$ – the dimensionless coordinate.

3. The definition of the criterion of explosive ignition by the electron beam with Gaussian distribution of energy along the beam cross-section

Based on the condition that as the result of the chemical energy in the solid, the rate of heat gain on the border of the reaction volume is equal to the rate of heat removal from the reaction layer deep into the explosive $Q_+ = Q_-$, according to paper [3], the heat balance equation is:

$$\pi r_1^2 \Delta z_1 \rho Q Z \exp\left(-\frac{E}{RT_m}\right) = -\lambda \pi r_1^2 \left(\frac{\partial T_1}{\partial z}\right)_{r=0, z=z_1} - 2\lambda \pi r_1 \Delta z_1 \left(\frac{\partial T_1}{\partial r}\right)_{z=z_m, r=r_1}, \quad (2)$$

where T_1 – the temperature on the border of the reaction volume; Δz_1 – the thickness of the reaction volume; r_1 – the radius of the reaction volume; Q – the thermal effect of the reaction on the mass unit of the explosive; Z – the frequency factor; E – the energy of the reaction rate activation; R – the gas constant.

Fig. 1a and Fig. 1b illustrate the qualitative dependence of normal (a) and radial (b) distribution of the density of the absorbed beam energy in the sample. The thickness of the reaction volume, according to Fig. 1a, is $\Delta z_1 = |z_1 - z_m|$, and it is defined by the equation [1]:

$$\Delta z_1 = R_{ef} \left(-\frac{2RT_m T_1 \Lambda_m}{E \Delta T_m \Lambda_m''} \right)^{1/2}, \quad (3)$$

where $\Lambda_m'' = \partial^2 \Lambda_m / \partial \xi^2$ – the second derivative of $\Lambda(\xi)$ at $\xi = \xi_m$ ($\Lambda_m'' < 0$).

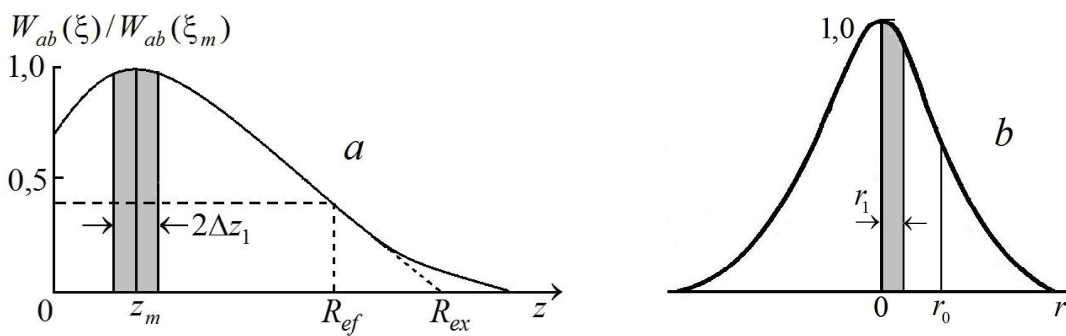


Figure 1. The qualitative dependence of normal (a) and radial (b) distribution of the density of the absorbed beam energy in the sample.

The temperature on the border of the reaction volume, defined on the condition that $Q_+(0)/Q_+(z_1) = e$, is [2]:

$$T_1 = \frac{T_m}{1 + RT_m / E}. \quad (4)$$

The distribution of the temperature along the sample at the pulse decay is defined by the expression

$$T(\xi, r) = T_0 + \frac{W}{c\rho R_{ef}} \Lambda(\xi) \exp\left(-\frac{r^2}{r_0^2}\right). \quad (5)$$

According to paper [1], the first derivative on the right side of the formula (2) is

$$\left(\frac{\partial T_1}{\partial z}\right)_{\substack{r=0 \\ z=z_1}} = \frac{W}{c\rho R_{ef}} \frac{\Delta z_1}{R_{ef}^2} \Lambda_m'' = \frac{\Delta T_m}{\Lambda_m} \frac{\Delta z_1}{R_{ef}^2} \Lambda_m''. \quad (6)$$

It is assumed that

$$\Delta T_m = T_m - T_0 = \frac{W}{c\rho R_{ef}} \Lambda_m. \quad (7)$$

Let us define the radial derivative on the right side of the formula (2). From expression (5) and (7) we have:

$$\left(\frac{\partial T}{\partial r}\right)_{z=z_m} = -\frac{2r}{r_0^2} \frac{W}{c\rho R_{ef}} \Lambda_m \exp\left(-\frac{r^2}{r_0^2}\right) = -\frac{2r}{r_0^2} \Delta T_m \Lambda_m \exp\left(-\frac{r^2}{r_0^2}\right).$$

Hence,

$$\left(\frac{\partial T_1}{\partial r}\right)_{\substack{z=z_m \\ r=r_1}} = -\frac{2r_1}{r_0^2} \Delta T_m \Lambda_m \exp\left(-\frac{r_1^2}{r_0^2}\right). \quad (8)$$

Let us define the radius of the reaction volume. According to (5) and (7), the expression for the temperature T_1 on the perimeter of the reaction volume at $\xi = \xi_m$ and $r = r_1$ is given by

$$T_1(\xi_m, r_1) = T_0 + \Delta T_m \exp\left(-\frac{r_1^2}{r_0^2}\right). \quad (9)$$

According to (9), the expression for the radius of the reaction volume is

$$r_1 = r_0 \ln\left(\frac{\Delta T_m}{T_1 - T_0}\right)^{1/2} = r_0 \ln\left(\frac{1 + \gamma}{1 - \gamma T_0 / \Delta T_m}\right)^{1/2}. \quad (10)$$

By substituting the derivatives (6) and (8) into the expression (2) and taking the account of the expression (10) for r_1 , after some transformation we get the criterion of explosive ignition by the pulsed electron beam, which includes the correction for radial heat removal from the area of electron absorption:

$$\rho Q Z \exp\left(-\frac{E}{RT_m}\right) = \frac{\lambda \Delta T_m}{R_{ef}^2} \left[-\frac{1}{\Lambda_m} \frac{\partial^2 \Lambda_m}{\partial \xi^2} + \frac{4}{F(\gamma)} \frac{R_{ef}^2}{r_0^2} \right]. \quad (11)$$

where $\gamma = RT_m / E$, and the function $F(\gamma) = (1 + \gamma) / (1 - \gamma T_0 / \Delta T_m)$. It should be noted, that due to the scattering the beam radius in the solid is to depend on z coordinate. That's why, the obtained criterion of explosive ignition by the electron beam, depending on the beam radius, is approximate.

The critical energy density for explosive ignition by the electron beam, taking into account the melting heat, is defined, based on the energy conservation law, by the formula:

$$W^* = \rho R_{ef} (c \Delta T_m + H_f). \quad (12)$$

4. The estimation of the effective track length of electrons

Major energy losses at the beam deceleration in the solid are ionizing. The curve of energy losses in the solid on the unit of track is normalized to the energy losses on the unit of track with energy E_0 , where E_0 is the initial kinetic energy of electrons.

The experimental curve, which reflects the distribution of absorbed energy density by the solid $W_{ab}(z)$, is often approximated by the cubic [5-6]:

$$W_{ab}(x) = f(z/R_{ex})W, \quad f(z/R_{ex}) = a + b(z/R_{ex}) + c(z/R_{ex})^2 + d(z/R_{ex})^3. \quad (13)$$

where R_{ex} – the extrapolated track length of the electrons; a, b, c – adjustable coefficients, which are defined on the condition of the best description of the experimental curve of the absorbed energy distribution. The function $f(z/R_{ex})$ has the maximum ($f_{\max} > 1$), and the integral is

$$\int_0^{R_{ex}} f(z/R_{ex}) dz = 1.$$

If the experimental curve of the absorbed energy distribution is normalized to the value of the density of the energy, absorbed at the maximum $W_{ab}(z_m)$, the expression (13) can be transformed as

$$\frac{f(z/R_{ex})}{R_{ex}} = \frac{f_{\max}}{R_{ex}} \left[a' + b' \left(\frac{z}{R_{ex}} \right) + c' \left(\frac{z}{R_{ex}} \right)^2 + d' \left(\frac{z}{R_{ex}} \right)^3 \right], \quad (14)$$

where $a = a'f_{\max}$, $b = b'f_{\max}$, $c = c'f_{\max}$, $d = d'f_{\max}$. Assume that $R_{ex}/f_{\max} = R_{ef}$. According to the agreed notations, the formula (14) goes as

$$\frac{f(z/R_{ex})}{R_{ex}} = \frac{1}{R_{ef}} \left[a' + \frac{b'}{f_{\max}} \left(\frac{z}{R_{ef}} \right) + \frac{c'}{f_{\max}^2} \left(\frac{z}{R_{ef}} \right)^2 + \frac{d'}{f_{\max}^3} \left(\frac{z}{R_{ef}} \right)^3 \right].$$

We write the function in brackets in dimensionless coordinates:

$$W_{ab}(\xi)/W_{ab}(\xi_m) = \Lambda(\xi) = a'' + b''\xi + c''\xi^2 + d''\xi^3.$$

Where constants $a' = a''$, $b' = b''/f_{\max}$, $c' = c''/f_{\max}^2$, $d' = d''/f_{\max}^3$.

Let us calculate the effective track length of electrons for PETN, depending on the kinetic energy of electrons. PETN is known to be a wide-band gap insulator [7]. The empiric formula for the evaluation of the extrapolated track length of electrons in explosives is given in paper [8]:

$$R_{ex} = \frac{a_1}{\rho} \left[\frac{1}{a_2} \ln(1 + a_2 e_0) - \frac{a_3 e_0}{1 + a_4 e_0^{a_5}} \right], \quad (15)$$

Here, ρ – the medium density, g/cm^3 ; $e_0 = E_0/mc^2$ – the medium relative kinetic energy of electron in the beam of high-current accelerator (mc^2 is the rest energy of the electron, equal to 511 keV); a_i – constants, depending on the effective atomic mass of the substance A_{ef} and the effective atomic number Z_{ef} . Constants a_i are calculated by the empiric formulae: $a_1 = 0,2335 A_{ef} / Z_{ef}^{1,209}$, $a_2 = 1,78 \cdot 10^{-4} Z_{ef}$, $a_3 = 0,989 - 3 \cdot 10^{-4} Z_{ef}$, $a_4 = 1,468 - 1,18 \cdot 10^{-2} Z_{ef}$, $a_5 = 1,232 / Z_{ef}^{1,209}$.

The effective atomic mass and the effective atomic number are defined by the following formulae

$$Z_{ef} = \sum_{i=1}^n f_i Z_i, \quad A_{ef} = \frac{Z_{ef}}{(Z/A)_{ef}}, \quad (Z/A)_{ef} = \sum_{i=1}^n (f_i Z_i / A_i), \quad f_i = A_i / \sum_{i=1}^n A_i.$$

Here, Z_i , A_i – the atomic number and the atomic mass of the i element; f_i – its weight fraction; n – the number of weight fractions.

The experimental curve of distribution of the absorbed energy for PETN [9] is satisfactorily described by the expression [10-12]:

$$W_{ab}(\xi)/W_{ab}(\xi_m) = \Lambda(\xi) = 0,7 + 1,57\xi - 2,31\xi^2 + 0,61\xi^3. \quad (16)$$

For PETN the electron track at the electron energy $E_0 = 250$ keV is $R_{ef} = 173,6 \cdot 10^{-4}$ cm, and $R_{ex} = 1,44R_{ef} = 250 \cdot 10^{-4}$ cm. The evaluation of R_{ef} for PETN, using the formula (15), at $\xi_{ex} = 1,44$ showed, that the calculated value of R_{ef} is approximately 14% smaller than R_{ef} , calculated on the experiment. That's why, the calculated values of R_{ef} for PETN at $E_0 = 450$, 600 and 1000 keV were increased by 14%, respectively. The calculation results are given in the table.

It should be noted that in reality the spectrum of electrons in the beam of a high-current accelerator is not monochromatic. There are electrons with energy, ranging from tens of keV to the value, corresponding to the amplitude of accelerating voltage [13], in the energy spectrum. So, the extrapolated track length of electrons is to be defined by the most high-energy electrons, and not by the medium kinetic energy. Naturally, the obtained criterion of condensed explosive ignition (11) doesn't take the account of nonmonochromaticity of the electrons in the beam of the high-current accelerator.

Table 1. The dependence of the effective track length of the electrons in PETN on the kinetic energy of electrons

E_0 (keV)	250	450	600	1000
$R_{ef}, 10^{-4}$ (cm)	173,4	414,7	624,6	1247

5. Calculation results

The calculations of the critical energy of PETN ignition by the electron beam were carried out at the following thermophysical and kinetic parameters: $c = 1255,2$ J/(kg·K), $\rho = 1,77 \cdot 10^3$ kg/m³, $\lambda = 0,2508$ W/(m·K), $H_f = 193$ kJ/kg, $E = 196,6$ kJ/mol, $Z = 6,3 \cdot 10^{19}$ s⁻¹, $Q = 1,26$ MJ/kg [14-16]. Fig. 2 *a*. shows the results of calculations for the critical density of the electron beam energy W^* for PETN, depending on the beam radius r_0 and the initial kinetic energy of electrons. According to the calculation data, presented in fig. 2 *a*, radial heat removal is to influence the critical energy density of explosive ignition by the electron beam only if the electron energy is $E_0 \sim 1000$ keV and the beam radius is $r_0 \sim 1$ mm. Fig. 2 *b* illustrates the calculation results for the critical energy density, determined using the formulae (11) and (12) depending on the initial electron energy in the pulse.

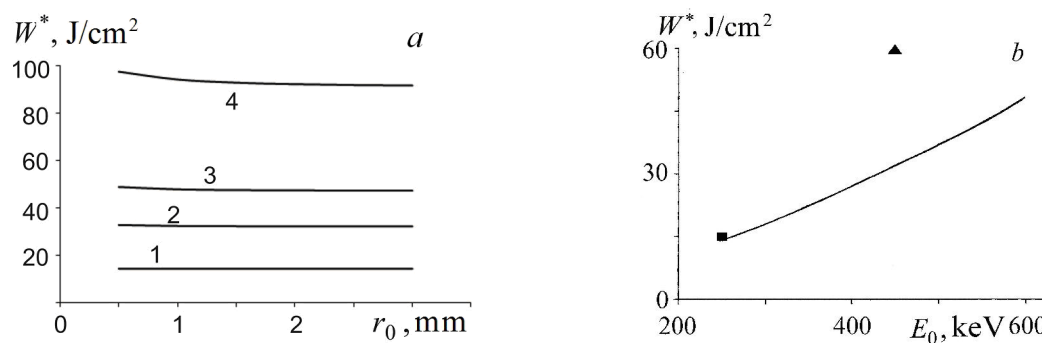


Figure 2. The dependence of critical energy density on the beam radius at different values of the beam energy for PETN: 1 – $E_0 = 250$; 2 – $E_0 = 450$; 3 – $E_0 = 600$; 4 – $E_0 = 1000$ keV (*a*) and the dependence of the critical density of the absorbed electron energy while PETN initiation on the initial electron energy in the beam: line – the calculation on the criterion (11) at $r_0 = 1$ mm; ■ – the experiment [9]; ▲ – the threshold energy of PETN detonation [17] (*b*).

As it is shown in fig. 2 *b*, the experimental value of the energy density of PETN initiation by the electron beam at $E_0 = 250$ keV [9] is in good agreement with the calculation. The density of the electron beam energy W_D ($E_0 = 450$ keV), at which the detonation of the explosive takes place [17], exceeds twice the critical value. In general, the calculation values of the density of the electron beam energy for PETN initiation by the electron pulse agree with and the experimental data quite satisfactorily, which proves the thermal mechanism of PETN initiation by a nanosecond electron beam.

The research has been carried out within the framework of the government contract № 3.1235.2014 K in the domain of science.

6. References

- [1] Khanef A V 1998 Criteria for ignition of condensed materials by an electron pulse *Chem. Phys. Reports*. **17**(8). 1573
- [2] Kovalskii A A, Khlevnoi S S and Mikheev V F 1967 The ignition of ballistite powders *Combust., Expl., Shock Waves*. **3**(4). 323
- [3] Khanef A V 1998 Effect of light distribution in the laser beam on the critical ignition energy of condensed materials *Chem. Phys. Reports*. **17**(10). 1889
- [4] Morozov V A, Savencov G G, Bragin V A, Kats V M and Lukin A A 2012 Problems in initiating detonation of disruptive explosives by a high-intensity electron beam *Technical Physics* **57**(5). 706
- [5] Harbeke G 1985 *Polycrystalline semiconductors. Physical Properties and Applications* (Springer-Verlag, Berlin, Heidelberg, New York, Tokyo)
- [6] Shiller Z, Gayzich U and Pancer Z 1980 *Elektronno-luchevaya tekhnologiya* (Moscow: Energija)
- [7] Zhurova E A, Stash A I, Tsirelson V G 2006 Atoms-in Molecules Study of Intra- and Intermolecular Bonding in the Pentaerythritol tetranitrate Crystal *J. Am. Chem. Soc.* **128**. 14728
- [8] Tabata T and Ito R 1974 An algorithm for the energy deposition by fast electrons *Nuclear Science and Engineering*. **53**. 226
- [9] Aduiev B P, Belokurov G M, Grechin S S and Shvaiko V N 2007 Investigation of the early stages of explosive decomposition of PETN crystals initiated by pulsed electron beams *Izv. Vyssh. Uchebn. Zaved., Fiz.* **50**(2). 3
- [10] Khanef A V, Duginov E V and Ivanov G A 2012 Modeling of PETN initiation by an electron beam with nanosecond duration *Khimicheskaya Fizika I Mezoskopiya*. **14**(1). 28
- [11] Khanef A V, Dolgachev V A, Duginov E V and Ivanov G A 2013 Criteria of energetic materials ignition by short laser and electron pulses *Bulletin of Kemerovo State University* **3**(55). 31
- [12] Ivanov G A and Khanef A V 2013 Radiation-thermal mechanism of initiation of PETN in the region of absorption of a nanosecond-duration electron beam *Russian Journal of Physical Chemistry B*. 2013. **7**(6). 741
- [13] Kulikov V D 2004 Electrification of high-resistance materials in high-power pulsed radiation fields (Tomsk: TGU)
- [14] Orlenko L P 2002 *Explosion Physics* (Moscow: Nauka)
- [15] Borisov A 1981 *Detonation and Explosives* (Moscow: Mir)
- [16] Baum F A, Derzhavec A S and Sanasaryan N N 1969 *Thermoresistant explosives and their effect in deep wells* (Moscow: Nedra)
- [17] Oleshko V I, Korepanov V I, Lisitsyn V M, Skripin A S and Tsipilev V P 2012 Electric breakdown and explosive decomposition of PETN monocrystals initiated by electron beam *Technical physics letters*. **38**(5). 415