Numerical Analysis of Indirect Optical Initiation of PETN

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Abstract. This paper deals with the numerical simulation of indirect optical initiation of explosives. The numerical simulation in the work was based on a physico-mathematical model that has been shown to successfully describe the direct laser ignition of PETN in optical detonator and the shock-wave ignition of porous PETN. Obtained numerical results are in good agreement with experimental data.

Introduction
Indirect optical initiation of explosives is actual area of research [1–2]. Optical detonator consists of a laser focused onto metal layer and low density PETN. Typical experimental arrangement is presented in figure 1. Using the metal film allows to decrease the threshold energy of PETN initiation because of the energy absorption increasing.

![Figure 1. Typical description of the experimental arrangement: laser beam: 1–glass; 2–metal film; 3–microstructure low density PETN](image)

Experimental analysis of direct and indirect optical initiation of explosives was carried out in [1]. The authors used the laser which had the following parameters: the laser length $\lambda=1.06$ microns, duration of the laser impulse $\tau=30\div50$ ns. The PETN and thin Mn film were used in optical explosive device. Researchers measured the threshold energy of PETN initiation.
Experimental investigations of an indirect optical initiation of explosive were carried out with PETN by dispersion 8000 cm$^2$/g$^2$ and density 0.9 g/cm$^3$ in [2]. The laser was similar to one from [1]. A lot of various metal films were considered: Al, Mn, Zn, Mg, Ni and others. It has been shown, that the relations between the threshold energy of PETN initiation and the film thickness were qualitatively similar for all considered metals.

The aim of present work is numerical simulation of the indirect optical initiation of PETN.

1. Description of the theoretical model

The experiment considered in this work should be analyzed as a multiphysics phenomena consisting of different branches of physics: plasma physics, optic physics, physics of explosion and etc. These processes have essentially various times and spatial scales. So the numerical simulation of laser detonator is very complicated problem.

In this paper we use model including various phenomenological models of processes compaction, chemical reaction etc. Though this approach simplifies the description of various physical and chemical processes, it allows to numerically simulate the processes occurring in experiments. This model was previously developed for numerical simulation of direct optical initiation of explosive in [3]. A good agreement between numerical and experimental results was obtained. The detailed description of this model see in [3, 4].

We modify our model for description of indirect optical initiation of explosives. Modification of this model relates with numerical simulation of interaction between laser radiation and metal film.

This interaction leads to strong heating, fusion, substance vaporization, ionization and plasma formation [5, 6].

We consider the thermal effect of these processes. Such approach allows us to model process of interaction between laser radiation and metal films as an external non-stationary energy source [5, 7].

Let us to estimate the spatial distribution of laser absorption energy in metal film taking into account the following expression for thermal wave length $\tau_0 = \sqrt{\kappa / \pi}$, where $\kappa$ – factor thermal diffusivity [8]. The thermal wave passes 2 microns during duration of the laser impulse (40 ns). This is 10 times thickness of metal films. It allows to consider interaction of laser radiation with a metal film in approach of uniform heating:

$$Q = \frac{WA}{\kappa} e^{-a(t-x)^2}$$

where $h$—thickness of a film, $W$—density energy, $A$—factor absorption.

It is necessary to take into account that depth of laser irradiation absorption is larger than the thickness of a metal film. That is why we can take into account the explosive heating by laser impulse. However in the present work the assumption of film opacity is used.

Interaction between laser impulse and metal film leads to various phase transition in metal. We use the Tillotson wide-range EOS [9] for description of these effects:

$$P_1 = A\mu + B\mu^2 + \left(a + \frac{b}{w_0}\right)\rho e, \mu \geq 0 (I),$$

$$P_2 = A\mu + \left(a + \frac{b}{w_0}\right)\rho e e_i, \mu < 0, e < e_i (\ II),$$

$$P_3 = P_2 + \frac{(P_2 - P_1)(e-e_i)}{(e_{id}-e_i)}, \mu < 0, e_i \leq e < e_{id} (\ III),$$

$$P_4 = a\rho e + \left(\frac{b \rho e + A\mu e^x}{w_0}\right) - \omega \mu, \mu < 0, e \geq e_{id} (\ IV),$$

$$w_0 = 1 + \frac{e}{\psi} \left(\frac{\rho}{\rho_0}\right)^2, \mu = \frac{\rho}{\rho_0}, \eta = 1 - \frac{\rho_0}{\rho}.$$
where $A, B, a, b, \alpha, \beta, \varepsilon_d, \varepsilon_s, \lambda, \gamma$ – constants [9–11].

This system consists of the four related equations. Each of them describes behavior of metal on a phase diagram. The first equation is responsible for a substance condition under the compression, the second equation describes the behavior of substance under the expansion. The fourth equation describes behavior of gaseous condition substance, and the third equation is responsible for an intermediate condition between the second and fourth equation. The detailed description of this model is presented in [3].

The system of equations was solved using the algorithm developed analogically one from [12, 13]. The numerical grid is common for all materials. We can use the non-uniform grid. A zones of contact are ideal [14]. The conditions of free surface or rigid wall can be set on a boundary of numerical area. Vector values are calculate in cell vertices. Scalar values are defined in the centers of cells. Let’s us to describe the order of the numerical calculations. At the first step we calculate the specific volume of cells, the equations of compaction and the chemical reactions. Following step is calculation of speed nodes of cell. Next step deals with the calculation of internal energy taking into account the external energy sources. The last step is calculation of new coordinates values for all nodes and calculation of pressure using the EOS.

We numerically simulated a series of shock wave tests for correcting our model and for comparing the numerical results with experimental data [8].

2. Numerical results

We made our numerical calculation using the one-dimensional statement and free boundary surfaces. The size of numerical area was 200 microns. The size of glass substrate was 100 microns Remained 100 microns are distributed between explosive and a metal film. The uniform grid was set with step by 2 nanometers in the field of an arrangement of a metal film. The non-uniform grid was set in zones of explosive and glasses for calculation acceleration. The explosive zone has 5000 cells and the glass zone has 1000 ones.

We varied the thickness of a film (from 20 nm to 160 nm with step by 20 nm) and laser energy (from 15 to 25 mJ with step by 0.5 mJ). Duration of a laser pulse was 40 ns ($\tau = 20$). The absorption factor was order of 0.4÷0.5 [2, 15]. Density explosive was 900 kg/m$^3$.

Uniform heating of a metal film increases the internal energy and pressure. At achievement of basic power points EOS of metal, there are changes of a phase condition of matter, and in both directions the waves leading compaction of explosive and its chemical decomposition start to extend. The further increasing of pressure causes the chemical reaction acceleration and the detonation wave formation on some distance from a film.

In figure 2 profiles of physical values are presented at the detonation process development in the system ($E = 21.5$ mJ, $h = 340$ nm, $A = 0.4$) with molybdenum film. Analyzing the profile density we can see the area with low values (less than 10 kg/m$^3$), showing strong expansion of a molybdenum film for the account a gain of internal energy is observed. On the profile mass fraction are presented processes chemical decomposition of explosive. From drawing also it is visible, that the detonation wave is formed on some distance from area of influence of a source: at the moment of time 70 ns and on distance of near 0.06 mm from a contact zone full burning explosive with sharp growth pressure and density.

The initiation energy dependence on a film (Ni, Mo) thickness for several factor absorptions is presented in figure 3: $E = \omega r^2$, where $r$ – radius [2].

3. Discussion of results

The obtained result for threshold initiation energy is in qualitatively agreement with experimental data. Growth of energy of initiation to the right of an optimum thickness of a film is connected with the big power expenses for a warming up of a material and its transfer in a gaseous condition. Growth of energy of initiation to the left of a minimum is connected by that the substance of a film is warmed up quickly, but, in turn, quickly unloads and cools down at achievement of a gaseous condition.
Figure 2. Spatial profiles for density, pressure and mass fraction at different time moments.

Figure 3. Relationship between the critical initiation energy of PETN explosion in and thickness film for several metals. experiments (exp)–[2], lines–numerical simulation (in brackets coefficient absorption).
The variation of absorption factor shows its essential influence on result: if factor decrease on 0.1 (to 0.4), threshold energy decrease on the average on 5 mJ. It is known from experiments [15], that at achievement in a metal film of temperature of boiling, optical depth increases, that at modeling was not considered. Nevertheless one-dimensional statement with continuum approach do not allow to carry out the analysis of scattering of substance of a film during a time of explosive. Besides there is opened a question about interaction of substance of a film and explosive from the chemical both thermal sides, and influence of these processes on result.

**Conclusion**

The optical initiation of explosives is actual area of research [1, 2]. Numerical analysis of indirect optical initiation of explosive is carried out in this paper. We consider the optical device consisting of glass, metal film, low density PETN. We use previously developed code for numerical simulation of shock wave tests and direct optical initiation of explosive [3, 4]. This model was modified. Modification of this model deals with numerical simulation of laser radiation interaction with metal film. Obtained numerical results are in good agreement with experimental results.

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