PHOTOACOUSTIC PULSES IN LASER-IRRADIATED METALS : NUMERICAL SIMULATION

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Abstract

The thermal generation of the elastic waves is considered in laser-irradiated metal (Cu) with temperature dependencies of the equation of state, heat transfer and optical properties of material taken into account. The influence of these quantities on frequency, phase and amplitude of photoacoustic pulses is analyzed. It is shown that the temperature dependencies of equation of state and absorptivity have the major influence on the pulse amplitude. The pulse phase changes mainly under the influence of absorptivity variation.

1- INTRODUCTION

The action of laser radiation on absorbing media is accompanied by generation of acoustic fields carrying information on the nature of the processes taking place in the sub-surface layer. The mechanisms of acoustic effects differ greatly and are determined both by the parameters of the incident laser pulse (intensity G, energy release rate $\partial G/\partial t$ and duration τ) and by the properties of the medium being irradiated (the changing density ϱ, thermo-physical and optical properties).

The most well-known sources of acoustic disturbances in irradiated media are the effects of thermal expansion, phase transitions (melting, surface and volume evaporation), optical breakdown and processes of plasma formation [1-5].

Although pressure pulses in metals and semiconductors have been investigated in many studies [4-8], the influence of various factors on the shape and amplitude of opto-acoustic pulses has not yet been adequately described even for the case of ordinary thermal expansion. The problem of signals interpretation is of paramount importance for opto-acoustic diagnostics.

2- The statement of the problem

A free surface of a plain copper plate is affected by a laser pulse of the intensity of 10-100 MW/cm^2 and a nanosecond duration. The radiation energy is absorbed in a thin subsurface layer, which results in a rapid heating of this layer. Due to thermal expansion, a pressure pulse appears in the heat affected zone and it propagates inside the material. The focal spot radius $r \gg \sqrt{a\tau_L}$, where a is the coefficient of thermal diffusivity, and the intensity distribution across the irradiated zone is taken to be uniform, therefore the problem is considered to be one-dimensional and it is only the longitudinal opto-acoustic pulses that are under study.

In order to describe the formation and propagation of an opto-acoustic signal, the full system of hydrodynamic equations is used, including the continuity equation, the momentum equation and the full energy equation accounting for the convective and conductive heat transfers. The system is supplemented with the necessary equations of state and the initial and boundary conditions.

We shall use the following system of notation that is standard for the given class of problems :
ϱ: density g/cm^3; u: velocity cm/s; p: pressure Bar; ε: internal energy J; T: temperature K; λ: thermal conductivity W/cm K; C_p: specific heat at constant stress J/g K; β: thermal expansion coefficient 1/K; A: absorptivity %; G_0: maximum intensity of laser radiation W/cm^2; τ_L: half-width of laser pulse ns; u_c: sound velocity in copper cm/s; l_T: thermal influnence depth cm.

Being reduced to the divergent form the system can be written in the following way :

$$\frac{\partial \varrho}{\partial t} + \frac{\partial}{\partial x}(\varrho u) = 0$$

$$\frac{\partial}{\partial t}(\varrho u) + \frac{\partial}{\partial x}(\varrho u^2) = -\frac{\partial p}{\partial x} \qquad (1)$$

$$\frac{\partial}{\partial t}\left(\varrho\left(\varepsilon + \frac{u^2}{2}\right)\right) + \frac{\partial}{\partial x}\left(\varrho u\left(\varepsilon + \frac{u^2}{2}\right)\right) = -\frac{\partial}{\partial x}(pu) + \frac{\partial}{\partial x}\left(\lambda(T)\frac{\partial T}{\partial x}\right)$$

$$x = [0, L], \qquad t = [t_0, t_1].$$

The equations of state are written as :

$$\varepsilon(\tau) = C_p(T)T$$

$$p(\varrho,T) = p_0\left(\left(\frac{\varrho}{\varrho_0} - 1\right) + \beta(T - T_0)\right) \qquad (2)$$

Note that the simplest relations are used as the equations of state. In a more general case to write the equation of state for a solid body with widely varying parameters is a difficult task. To resolve this task, special calculation techniques can be applied.

The initial and boundary conditions are as follows :

$$t = t_0 : \varrho = \varrho_0, \; u = 0, \; T = T_0;$$

$$x = 0:$$

$$p = 0, \; -\lambda \frac{\partial T}{\partial x} = G(t), \; G(t) = A(T) G_0 \exp\left(-\frac{t}{\tau_L}\right)^2; \tag{3}$$

$$x = L: \quad u = 0, \; \lambda \frac{\partial T}{\partial x} = 0.$$

The major object of the study is the dependence $P(t)$ (i.e. the value of pressure versus time) at the surface $x = x_p$ which may coincide with the boundary $x = L$ or be positioned inside the plate : $P(t)=p(x=x_p, t+\tau)$. The parameter $\tau = x_p / u_s$ denotes the time delay of the observed acoustic pulse as compared with the laser pulse. This delay is connected with the propagation time of a thermo-dynamic disturbance down to the depth x_p where the pulse is observed.

3- ANALYSIS OF THE RESULTS

Let us consider and analyze changes in the amplitude and frequency characteristics of the opto-acoustic pulse associated with the temperature dependencies of the equation of state and thermo-physical $\lambda(T)$, $C_p(T)$ and optical $A(T)$ properties of the metal. In most metals, as the temperature rises, the specific heat and absorptivity increase and the thermal conductivity decreases. As for changes in the equation of state, for the simplest case under discussion they can be reduced to acceleration and deceleration of thermal expansion. For numerical modeling the relations typical of copper will be used.

$$\begin{array}{lll} A(T) = A_0(1+K_A \Delta T), & A_0 = 0.05, & K_A = 2.8.10^{-3}; \\ C_p(T) = C_{p0}(1+K_c \Delta T), & C_{p0} = 0.396, & K_c = 2.1.10^{-4}; \\ \lambda(T) = \lambda_0(1-K_{\lambda} \Delta T), & \lambda_0 = 4.02, & K = 2.4.10^{-4}; \\ \varrho(T) = \varrho_0(1-\beta_0 \Delta T), & \varrho_0 = 8.56, & \beta_0 = 6.72.10^{-5}. \end{array} \tag{4}$$

where ΔT is the temperature increment, $\Delta T = T - T_0$, T_0 is room temperature. In some calculations the following temperature dependence for the thermal conductivity will also be used :

$$\lambda_5(T) = \begin{cases} \lambda_0(1-5K \Delta T), & T \leq 860 \text{ K} \\ 0.33\lambda_0, & T > 860 \text{ K} \end{cases} \tag{5}$$

In all the calculations the laser pulse half-width was $\tau_L = 50$ ns and the intensity varied within the range $G_0 = 10^7 \div 10^8$ W/cm^2. At such action parameters the calculated surface temperature did not exceed the melting point $T_m = 1356$ K for copper. In this case the maximum temperature increment was $\Delta T = T_{melt} - T_0 = 1056$ K, and the greatest possible deviations of the values of the coefficients from those at room temperature are :

$$A_{max} \simeq 3.0A_0, \quad C_{p,max} \simeq 1.25C_{p,0}, \qquad \lambda_{min} \simeq 0.75\lambda_0, \quad \lambda_{5,min} \simeq 0.33\lambda_0. \tag{6}$$

The relations (6) indicate that when the dependencies (4) typical of copper are used, a relative change in absorptivity is about one order higher than relative changes in thermal conductivity and specific heat. On the other hand, the dependence of thermal conductivity (5) is given in such a way that, as the temperature rises, its value decreases by so many times as the absorptivity value increases.

Opto-acoustic pulses were analyzed according to the following scheme. Each characteristic under study (A_0, C_{p0}, λ_0, β) may be either constant or linearly dependent on temperature. An acoustic pulse corresponding to constant values at a given intensity is taken to be basic and assigned the index 0. Then by varying one or several parameters and the intensity G_0 and comparing opto-acoustic pulses with the basic one and with each other, we study the influence of these parameters.

THE INFLUENCE OF THERMO-PHYSICAL PROPERTIES. Analysis of the influence of parameters variations begins with the thermal dependencies of the coefficients of thermal conductivity and specific heat. Consider the following sets of dependences :

$$\begin{aligned} i = 0&: \quad A = \text{const},\ C_p = \text{const},\ \lambda = \text{const}; \\ i = 1&: \quad A = \text{const},\ C_p = C_p(T),\ \lambda = \lambda(T); \\ i = 2&: \quad A = \text{const},\ C_p = C_p(T),\ \lambda = \lambda_5(T). \end{aligned} \tag{I}$$

For each set the calculation is made at $G = 7.10^7\ W/cm^2$ $G = 10^8\ W/cm^2$. The dependencies of temperature and pressure are presented in Fig. 1.

On the basis of the calculations at i = 0,1,2 one can come to the conclusion that temperature changes of thermal conductivity and specific heat, being typical of metals, do not affect the frequency and phase parameters of the pulse, but do affect the pulse amplitude by reducing it by 10-40%. The weakening effect of specific heat is greater than that of thermal conductivity and the amplitude of the minimum is decreased greater than that of the maximum.

THE INFLUENCE OF ABSORPTIVITY. Now we shall analyze the response of an opto-acoustic pulse to the temperature dependence of absorptivity and compare it with the effect of thermo-physical properties. The set of the calculation results (group II) at the same values of the intensity $G=7.10^7\ W/cm^2$ and $G=10^8\ W/cm^2$ as used for group (I) is presented in Fig. 2.

$$\begin{aligned} i = 3&: \quad A = A(T),\ C_p = \text{const},\ \lambda = \text{const}; \\ i = 4&: \quad A = A(T),\ C_p = C_p(T),\ \lambda = \lambda(T); \\ i = 5&: \quad A = A(T),\ C_p = C_p(T),\ \lambda = \lambda_5(T). \end{aligned} \tag{II}$$

On the whole, the analysis carried out shows that when the ordinary dependencies of optical and thermo-physical properties (4) are used, the influence of increasing absorptivity on the amplitude is dominant, however in the case of extremely quick decrease of thermal conductivity, the

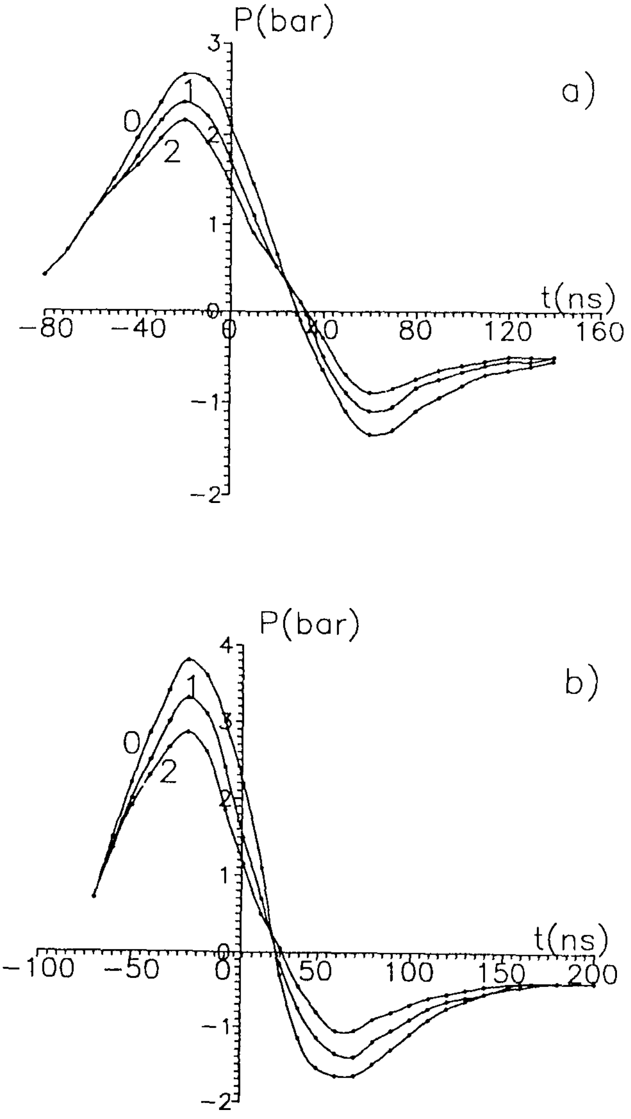

Fig.**1** . Photoacoustic pulses *P(t)* versus time : (a) - $G_0 = 7\ 10^7$ W/cm^2; (b) - $G_0 = 10^8$ W/cm^2; for all the curves $A = A_0$; curve 0 - $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 1 - $C_p = C_p(T)$, $\lambda = \lambda(T)$; curve 2 - $C_p = C_p(T)$, $\lambda = \lambda_s(T)$. The middle of laser pulse corresponds to $t = 0$.

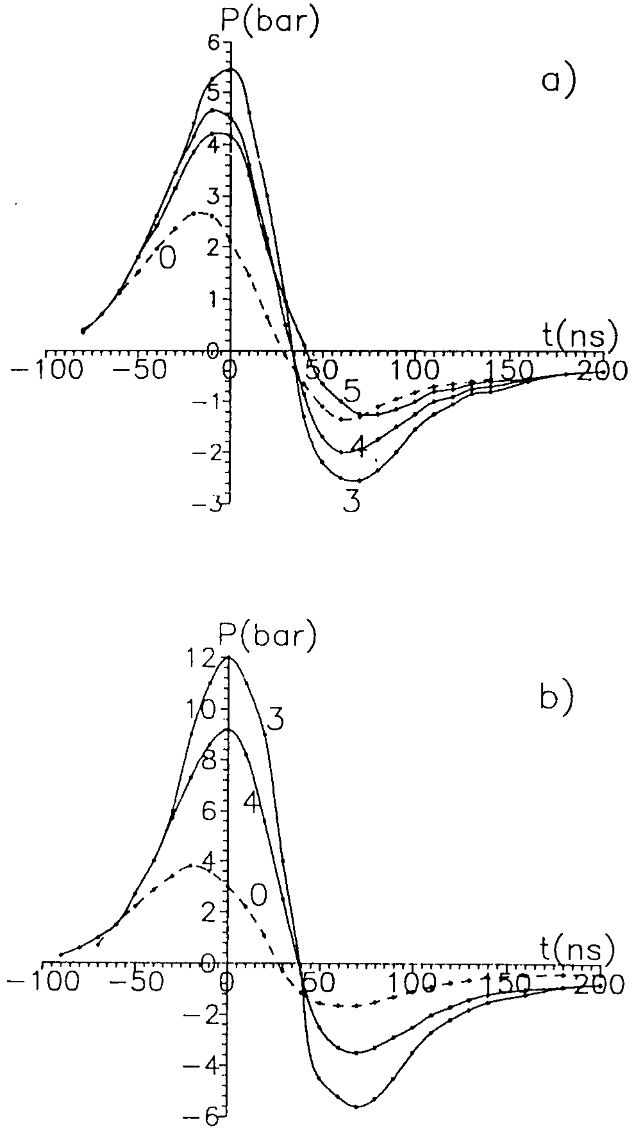

Fig. **2** . Photoacoustic pulses $P(t)$ versus time : (a) - $G_0=7\ 10^7$ W/cm^2; (b) - $G_0=10^8$ W/cm^2; for all the solid lines curves $A=A(T)$; curve 3 - $C_p=C_{p0}$, $\lambda=\lambda_0$; curve 4 - $C_p=C_p(T)$, $\lambda=\lambda(T)$; curve 5 - $C_p=C_p(T)$, $\lambda=\lambda_5(T)$; dashed line curve 0 - $A=A_0$, $C_p=C_{p0}$, $\lambda=\lambda_0$. The middle of laser pulse corresponds to $t=0$.

amplitude of the negative branch may remain unchanged.

THE INFLUENCE OF THE EQUATION OF STATE. Now we shall analyze the influence of temperature variations in the equation of state on the opto-acoustic pulse. Let us consider the simplest form of such changes and write two new equations of state, taking the coefficient β in the form of a steplike function with a gap at the point T^* :

$$p = p_0\left(\left(\frac{\varrho}{\varrho_0}-1\right)+\beta_1(T-T_0)\right),\ \beta_1=\beta_0\varkappa(T^*-T)+ 2\beta_0\varkappa(T-T^*); \qquad (8)$$

$$p = p_0\left(\left(\frac{\varrho}{\varrho_0}-1\right) + \beta_2(T-T_0)\right),\ \beta_2=\beta_0\varkappa(T^*-T)+ \frac{1}{2}\beta_0\varkappa(T-T^*); \qquad (9)$$

$T^* = 346$ K, $\varkappa(x)$ - is the Haviside unit function :

$$\varkappa(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}.$$

The physical meaning of the given equations is that, beginning from a certain temperature, thermal expansion of a body is accelerated or decelerated by a factor of two, respectively. The dependence of the equilibrium value of density $\varrho(T)$ for each equation of state (8) and (9) has a kink at the temperature $T=T^*$.

Let us first analyze the equation of state (8). The corresponding calculations were made at $G=8.10^7$ W/cm^2 and $G=10^8$ W/cm^2 for the following set of optical and thermo-physical parameters.

$$\begin{array}{llll} i = 1: & A = \text{const}, & C_p = \text{const}, & \lambda = \text{const}; \\ i = 2: & A = \text{const}, & C_p = C_p(T), & \lambda = \lambda(T); \\ i = 3: & A = A(T), & C_p = \text{const}, & \lambda = \text{const}; \\ i = 4: & A = A(T), & C_p = C_p(T), & \lambda = \lambda(T). \end{array} \qquad (III)$$

Fig. (3), shows the P(t) dependencies for group (III). Thus, the equation of state (8) increases selectively the pulse amplitude, changes slightly the value of the pressure maximum and to a considerable extent the value of the minimum. All of this gives the pulse, as a whole, a symmetrical bipolar form typical for strongly-conducting and strongly-absorbing media.

Now we shall pass on to study the effect of the equation of state (9). Calculations were made at the same intensities and the same sets of parameters as for the equation of state (8). The results are presented in Fig.4. On the whole, the results discussed indicate that the equation of state (9), as well as (8), affects the amplitudes of the two pulse branches in different ways : it slightly weakens the positive branch and very strongly weakens the negative one, its action in the latter case being dominant over those of other parameters. At a high intensity the negative branch becomes negligibly weak and the pulse becomes nearly unipolar, with the frequency being twice as great as that of the linear

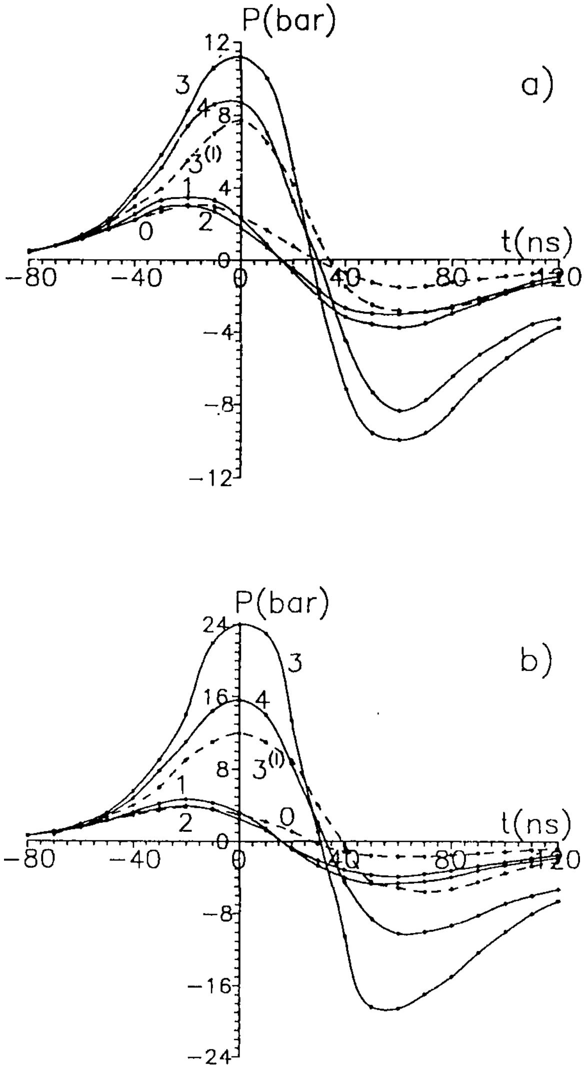

Fig. **3** . Photoacoustic pulses *P(t)* versus time : (a) - $G_0 = 8\ 10^7$ W/cm^2; (b) - $G_0 = 10^8$ W/cm^2;
for all the solid lines curves $\beta = \beta_1(T)$: curve 1 - $A = A_0$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 2 - $A = A_0$, $C_p = C_p(T)$, $\lambda = \lambda(T)$; curve 3 - $A = A(T)$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 4 - $A = A(T)$, $C_p = C_p(T)$, $\lambda = \lambda(T)$;
for all the dashed line curves $\beta = \beta_0$: **0** - $A = A_0$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 3′ - $A = A(T)$, $C_p = C_{p0}$, $\lambda = \lambda_0$.
The middle of laser pulse corresponds to $t = 0$.

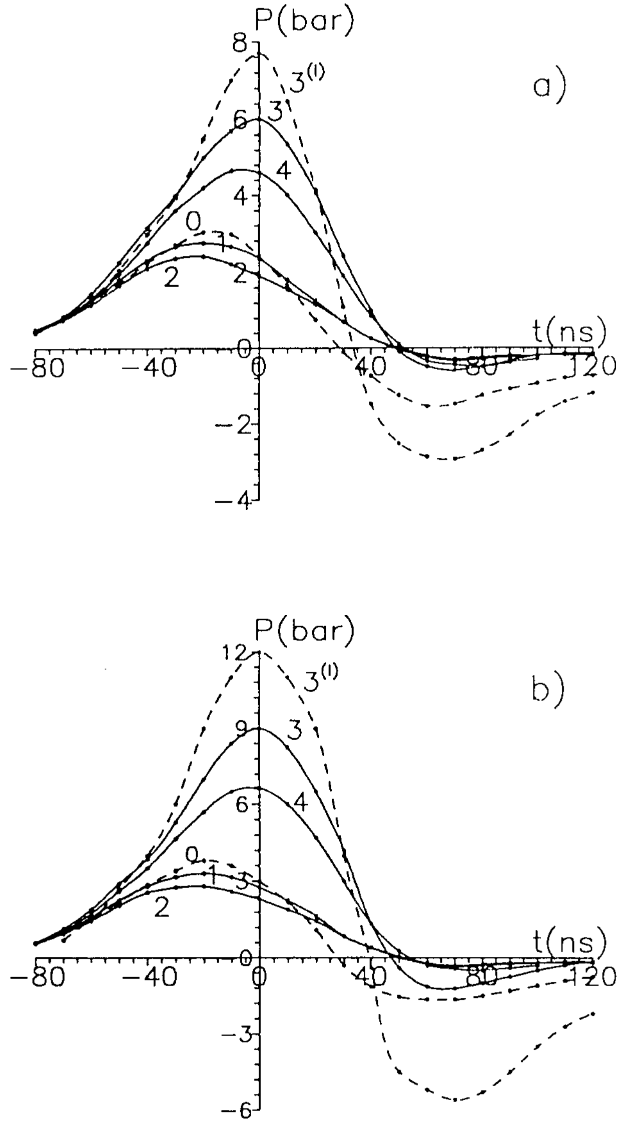

Fig.**4** . Photoacoustic pulses $P(t)$ versus time : (a) - $G_0 = 8\ 10^7$ W/cm^2; (b) - $G_0 = 10^8$ W/cm^2;
for all the solid lines curves $\beta = \beta_2(T)$: curve 1 - $A = A_0$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 2 - $A = A_0$, $C_p = C_p(T)$, $\lambda = \lambda(T)$; curve 3 - $A = A(T)$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 4 - $A = A(T)$, $C_p = C_p(T)$, $\lambda = \lambda(T)$;
for all the dashed line curves $\beta = \beta_0$: **0** - $A = A_0$, $C_p = C_{p0}$, $\lambda = \lambda_0$; curve 3′ - $A = A(T)$, $C_p = C_{p0}$, $\lambda = \lambda_0$.
The middle of laser pulse corresponds to $t = 0$.

pulse.

4- CONCLUSION

On the basis of the performed analysis it is possible to distinguish the following main characteristics of the opto-acoustic pulse response to the typical changes of thermophysical properties, absorptivity and equation of state.

1. Among the factors under study, the surface absorptivity A(T) and equation of state may exert the strongest influence upon the opto-acoustic pulse.

2. The equation of state, which models the acceleration of thermal expansion, makes the pulse symmetrically bipolar by increasing the pulse amplitude. In the case of decelerated expansion, the equation of state decreases the pulse amplitude, affecting mostly the negative branch of pressure and converting the pulse into nearly an unipolar one.

3. The increase of absorptivity, in addition to a considerable amplification of the pulse amplitude, changes the positive half-wave phase due to the fact that it takes more time to achieve the maximum pressure.

4. The increase of specific heat and the decrease of thermal conductivity do not affect the frequency and the phase of the pulse, but do attenuate the pulse.

5. The attenuating effect of thermo-physical properties cannot compensate the amplifying effect of absorptivity. A partial compensation takes place only in the case of a very quickly decreasing thermal conductivity.

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