Temperature dependence of the loss coefficients in the formation of laser-stimulated nanostructures

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Problem formulation

Contemporary lasers and laser systems generate femtosecond impulses (1 fs=10^{-15} s). Femtosecond laser systems with light impulse duration 10–1000 fs allow obtaining under focusing enormous light intensity over 10^{13} W/cm^2. After falling on solid matter surface such high intensity impulses can, under some conditions, lead to considerable damages of this surface. If the flow is substantially higher than critical value, considerable part of energy of laser radiation is outlaid on a direct phase solid-gas transition. A liquid phase in the area of treatment is practically absent in this case. Such streams represent the main interest of this research.
An updated system of two interrelated differential equations for the dimensionless dynamics of the crater shape function *S* and the dimensionless surface pressure *P* was obtained:

$$\frac{\partial S}{\partial t} = \frac{P^{\beta}}{L_d^2}\sqrt{1+\left(\frac{\partial S}{\partial r}\right)^2} \quad (1)$$

$$\frac{\partial P}{\partial t} = \frac{L_d^{2-\beta-\eta}}{L}\left(L\Lambda e_q \vartheta(\tau - t) - 1\right)P^{\beta+\eta} - \frac{L_d^{1-\beta}}{L}P^{\beta+1} + e_q\frac{L_d^{2-\eta}}{L}\frac{\vartheta(\tau-t)P^{\eta}}{\sqrt{1+(\partial S/\partial r)^2}}. \quad (2)$$

Here $\beta = (\kappa+1)/2\kappa$; $\eta = 1/\kappa$; $(1 < \kappa \leq 5/3)$; Λ and e_q – factors associated with the absorption of radiation by the plasma-gas phase; *t* is dimensionless time, and *r* is dimensionless radial spatial variable. This system describes the process of high precision laser surface treatment with crater formation but no melt formation. It differs from a similar system considered earlier in taking into account explicitly two phenomenological parameters: L_d and L, which are, respectively, the optical and thermal loss coefficients of the initial flow when it passes the surface to be treated.

Surface losses with powerful laser irradiation

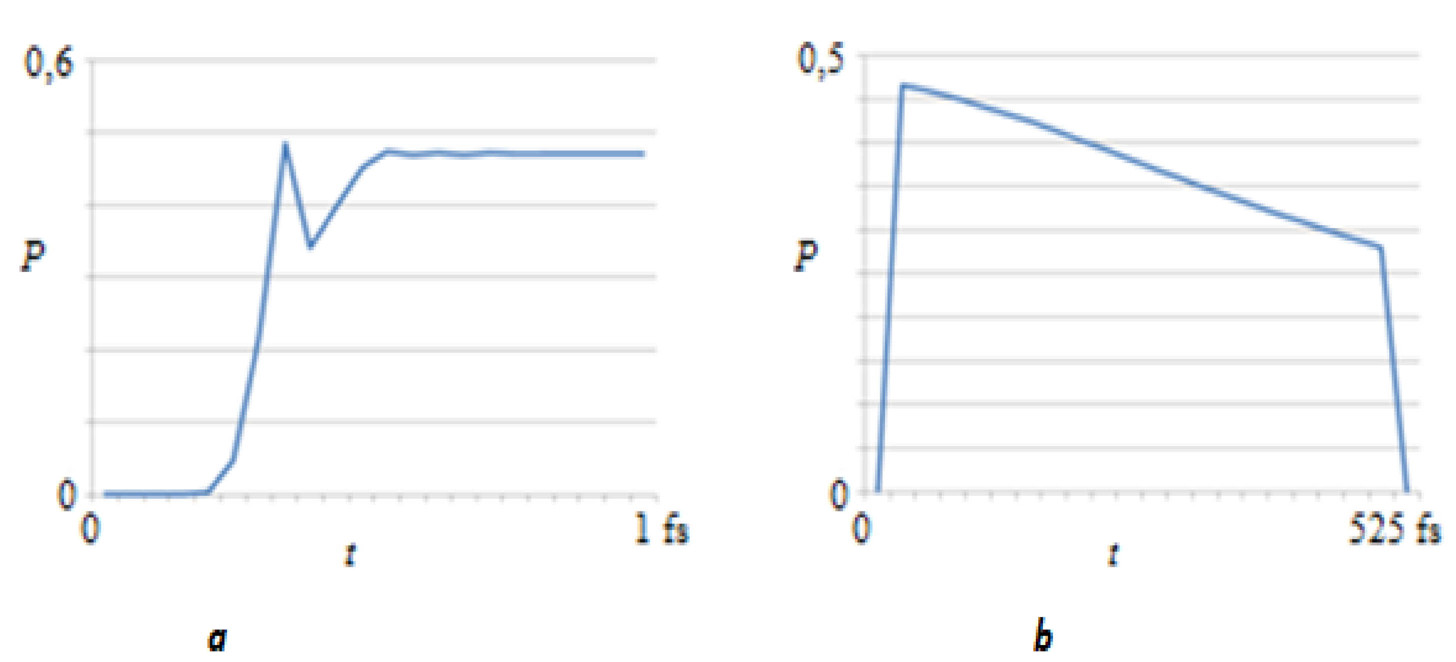

Fig. 1. Dependence of dimensionless pressure on time on the pulse axis at its maximum femtosecond duration of 500 fs at a radiation flux $(7\cdot 10^{15}\ \mathrm{W/m^2})$: (a) the initial stage of the process $t \leq 1\ fs$; (b) the whole process $t \leq 525\ fs$

In numerical modeling using a previously considered similar system, these coefficients were considered constant and taking values in the range from 0 to 1. At the same time, they were not explicitly included in the equations, since they were included in the parameters which are normalizing the values *S*, *P*, *t*, *r*. In this sense, there was no need to set the parameters L_d and L for dimensionless calculations. If there was a need to estimate the real values of *S*, *P*, *t*, *r*, then these coefficients were assumed to be 0.5. In particular, the carried out calculations for the case of dimensionless constants L_d and L determine the changes in pressure *P* (Fig. 1) during the formation of a crater. Тщательные исследования процессов, определяющих поверхностные потери, показали, что эти коэффициенты взаимосвязаны и существенно зависят от температуры. Именно это заставило переформулировать систему до вида (1), (2).
Прежде всего, установлено, что с высокой степенью точности выполняется соотношение: $L = 1 - L_d$. Действительно, с одной стороны, все оптические потери определяются двумя факторами: коэффициентом отражения *R* и процессами рассеяния, безразмерный фактор для которых обозначим через Σ. То есть, $L_d = R + \Sigma$. С другой стороны, убывание потока излучения q_s, дошедшего до поверхности, при прохождении самой поверхности, трансформируется до вида: $q_{in} = (1 - L_d)\cdot q_s$. А дальше в объеме материала убывает в соответствии с равенством: $q_{out} = q_{in}\cdot \exp(-k_0\cdot z) = (1-L_d)\cdot q_s \cdot \exp(-k_0 \cdot z)$, где k_0 – коэффициент поглощения излучения твердой фазой, z – глубина проникновения излучения в материал. Соответственно, часть потока излучения: $q_T = q_{in} - q_{out}$, поглощенная материалом и идущая на нагрев, имеет такой явный вид:

$$q_T = (1 - L_d)\cdot q_s \cdot [1 - \exp(-k_0\cdot z)]\ . \quad (3)$$

Принимая во внимание, что коэффициент поглощения многих материалов, особенно металлов, в хорошем приближении можно считать бесконечно большим, а коэффициент тепловых потерь *L* определяется соотношением: $L = q_T/q_s$, из равенства (3), с хорошей степенью точности, можно найти: $L = 1 - L_d$. Тогда в уравнении (2) все коэффициенты *L* можно заменить разностью $L = 1 - L_d$ и далее остановиться подробно только на коэффициенте L_d.
Как уже отмечалось:

$$L_d = R + \Sigma. \quad (4)$$

Temperature dependence of loss coefficients

As studies have shown the reflection coefficient depends on the temperature:

$$R = R_0 - \sqrt{\rho N_A}e/\left(\sigma_{el}\sqrt{\pi\mu m_e}\right) ln(T/T_0).$$

Without accounting scattering losses, optical losses are completely determined by reflection:

$$L_d = R_0 - e\sqrt{\rho N_A}/\left(\sigma_{el}\sqrt{\pi\mu m_e}\right) ln(T/T_0). \quad (5)$$

And the temperature, in turn, is determined by the equality:

$$T/T_0 = 1 + L_d\left(2q_{in}\sqrt{t_0}/\left(T_0\sqrt{\pi\lambda\rho C_v}\right)\right)\sqrt{t}, \quad (6)$$

and, as it seen, depends on L_d. That is, these two equalities are actually two related equations that require mutually consistent analysis. The results of this analysis are shown in Fig. 2 for parameter values corresponding to silver. In particular, was denoted: σ_{el} – electrical conductivity; μ – molecular weight; T_0 – initial temperature (293^oK); t_0 – parameter which normalized time to dimensionless form; λ - thermal conductivity; ρ is the density.
It can be seen from the graphs (Fig. 2a, 2c) that the critical temperature for silver $T_{cr} = 6000^o$K is reached already at the moment $t_{cr} \sim 0.57$ fs $(5.7\cdot 10^{-16}$ s). The moment t_{cr} can be estimated without the joint numerical implementation of the coupled pair of equations (5), (6). To do this, it is enough to put $T = T_{cr}$ in (5), (6), substitute (5) in (6) and solve (6) relatively to time *t*. With pulse duration ~ 140 fs, the achievement of the moment $t_{cr} \sim 0.57$ fs can be considered almost instantaneous. However, this period cannot be neglected, since this period forms the initial conditions for the numerical implementation of system (1), (2). Fig. 2b demonstrates a decrease in optical loss based on reflection only from 0.930 to 0.918 as the temperature rises from initial value to critical.
At the period before the moment of destruction appearance $(T < T_{cr})$, radiation losses on the small hemispherical irregularities (with a radius of up to 100 Å) were also analyzed. An analysis of the factor Σ on the scattering losses in definition (4) due to such irregularities leads to an insignificant change in the dependence 2b. The integral deviation of the curves does not exceed 0.03% towards an increase in L_d. Due to the smallness of the effect and the cumbersomeness of the formula for the factor Σ, this formula is not presented here.
After the beginning of destruction $(T > T_{cr})$, the reflection loss (5) takes on a value fixed at the temperature T_{cr}, and instead of scattering by irregularities, the scattering losses in the plasma-gas phase are switched on. Losses in it for absorption are already taken into account in system (1), (2) in the form of factors Λ and e_q. For silver, the ionization energy is so high $(\sim 80000^o$K) that practically no plasma is formed and the removal of matter from the solid phase occurs mainly in the form of non-ionized gas.

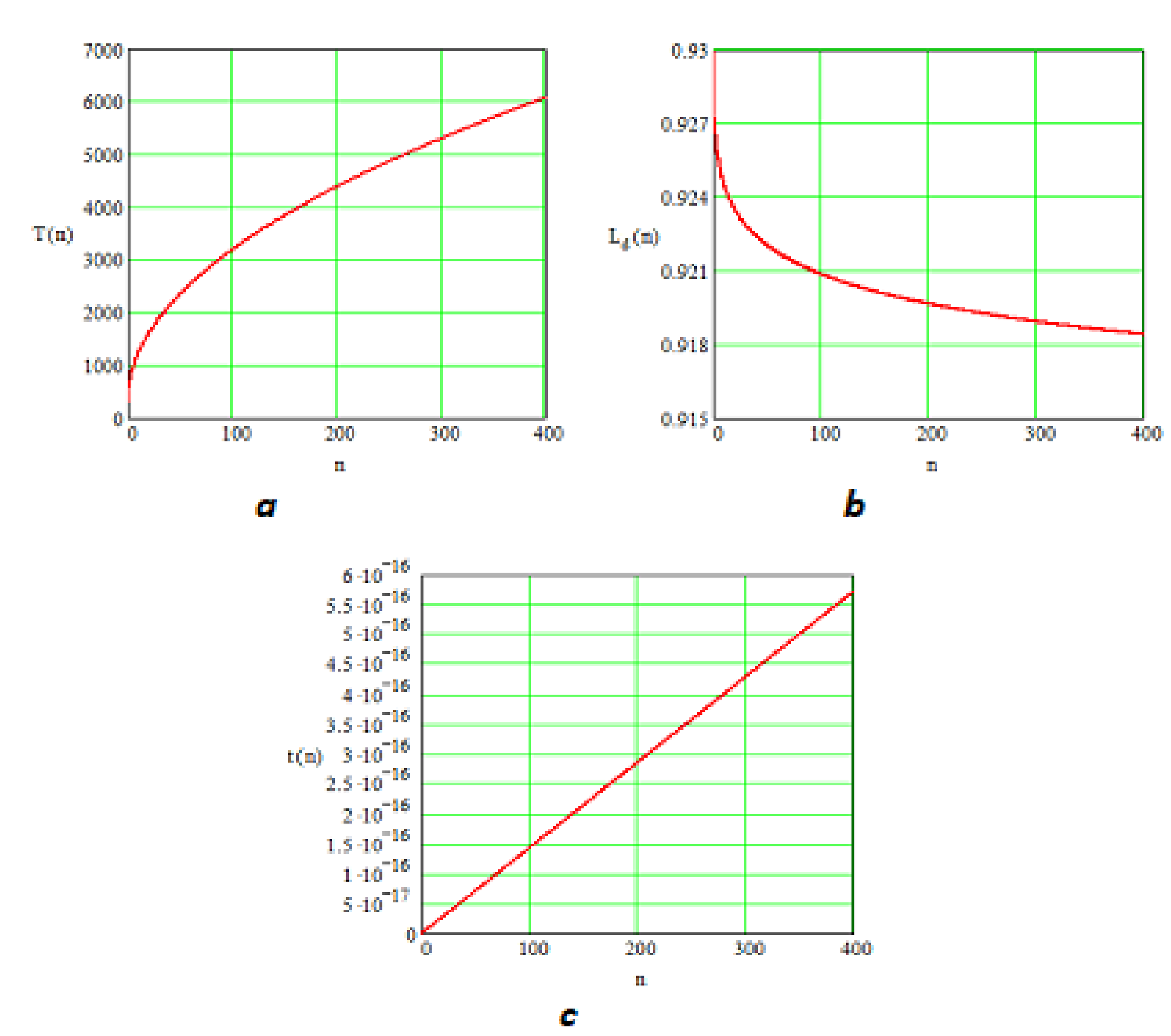

Fig. 2. Time dependence of temperature (graph a) and optical loss (graph b) (reflection only). The graph (c) is intended to translate the integer parameter n into real time (s). Here we also used the parameters for silver and the radiation flux $7\cdot 10^{15}\ \mathrm{W/m^2}$, but for a pulse duration ~ 140 fs, which is often used in real experiments.