

THE STUDY OF CLASSICAL HIGH POWER LASERS CALORIMETRY WITH APPLICATIONS ON THIN FILMS

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(Received January 7, 2008)

Abstract. In the present paper we are dealing with the thermal field for free electron laser-thin film interaction. We propose a simplified model which takes into account one global heat equation instead of two coupled heat equations. For parameters which are of the same order of magnitude we take into consideration just the thermal coefficients of the substrate. The idea of our model is to consider an absorption coefficient as close as possible to reality. We solve the heat equation using the integral transform technique. We plot the thermal field at the interface for different situations. Our results indicate that: (i) the thermal field depends strongly on the absorption coefficient of the thin film and (ii) the length of the interface, at least in the domain 0.1–10 μm does not play an important role in the thermal fields.

Key words: free electron laser, CO₂, substrate, thin film, heat equation, thermal field.

1. INTRODUCTION

Light has always played a central role in the study of physics, chemistry and biology. In the last century a new form of light, laser light has provided important contributions to medicine, industrial material processing, data storage, printing and defense [1]. In all this areas of applications the laser-solid interaction played a crucial role. For describing this interaction the classical heat equation was used in a lot of applications [2–9]. Apart of some criticism [10], the Fourier heat equation still remains a powerful tool for describing thermal effects in laser-solid interaction [11–15]. The heat equation can be used for describing both: interactions with homogeneous [16–19] and inhomogeneous solids [20–21]. Special attention was given for multi-layered samples [22–23] and thin films.

2. THE STATEMENT OF THE PROBLEM

Let us suppose that we have a solid which contains a substrate of Si and thin film consisting of one of the materials: Au, Ag, Al or Cu. Assuming that only photothermal action takes place, and that all absorbed energy was transformed into heat, the linear heat flow in the solid is fully described by the partial differential equation:

$$\frac{\partial^2 T(r, z, t)}{\partial r^2} + \frac{1}{r} \frac{\partial T(r, z, t)}{\partial r} + \frac{\partial^2 T(r, z, t)}{\partial z^2} - \frac{1}{\gamma} \frac{\partial T(r, z, t)}{\partial t} = -\frac{A(r, z, t)}{k}, \quad (1)$$

where: γ is the thermal diffusivity, k is the thermal conductivity and $A(r, z, t)$ is the volume heat source (per unit time). In general one can consider the linear heat transfer approximation [2, 17]. We will consider only the radiation case (we assume a zero convection): $h_{rad} = 4\sigma ET_0^3$ (σ is the Stefan-Boltzmann constant and E is the emissivity of the sample) and the following boundary conditions:

$$\begin{aligned} k_{1,2} \frac{\partial T_{1,2}(r, z, t)}{\partial r} \Big|_{r=a} + h \cdot T_{1,2}(a, z, t) &= 0, \\ k_1 \frac{\partial T_1(r, z, t)}{\partial z} \Big|_{z=b} + h \cdot T_1(r, b, t) &= 0, \\ k_2 \frac{\partial T_2(r, z, t)}{\partial r} \Big|_{z=c} + h \cdot T_2(r, c, t) &= 0. \end{aligned} \quad (2)$$

Here h is the heat transfer coefficient and $T(r, z, t)$ is defined here as the difference $T_{fi} - T_{in}$, where T_{fi} and T_{in} are the final and initial absolute temperatures of the sample.

This definition implies that: $T(r, z, 0) = 0$, which makes the Laplace transform more convenient than the Green function method [2].

We take the z direction as the laser propagation, a is the radius of the cylinder, b is the thickness of the substrate and c is the thickness of the thin film (we have considered a cylinder sample). In addition we have at the interface ($z = 0$):

$$k_1 \frac{\partial T_1(r, z, t)}{\partial z} \Big|_{z=0} = k_2 \frac{\partial T_2(r, z, t)}{\partial z} \Big|_{z=0}$$

and “cylinder” condition,

$$T_1(r, z, t) \Big|_{z=0} = T_2(r, z, t) \Big|_{z=0} \quad (3)$$

One can try to solve equation (1) with the boundary conditions (2) and (3). This however is a very difficult task, to get an analytical solution. On the other

hand it suppose that all thermal parameters of the sample must be described by step like functions (which is not necessary true, especially when we have a big differences between the thermal parameters). In the next chapter we will propose a model able to avoid this difficulties.

3. THE MODEL

The first approximation to consider is to calculate the thermal field considering only the substrate because: $c \ll |b|$, $b < 0$; c being of the order of magnitude of μm and b being of the order of magnitude of mm .

In order to make an approximation we have to analyze the thermal parameters of the substrate and thin films (Table 1). We will suppose that we do not have variation with temperature of the sample thermal parameters. For laser - thin film interaction the heat equation is valid for a length l , $l \geq 0.02 \mu\text{m}$.

Table 1

The thermal parameters for: Si, Cu, Al, Ag, Au

	K [W/cmK]	γ [cm^2/s]	α [cm^{-1}]
Si	1.5	0.85	50
Cu	3.95	1.14	7.7×10^5
Al	2.4	1.03	10^6
Ag	4.28	1.72	8.33×10^5
Au	3.15	1.22	7.7×10^5

In our model we will not consider the variation of the thermal parameters with temperature, because in this case we have no analytical solutions. One can observe that for k and γ we have the same order of magnitude. In consequence we can consider that we have one solid sample with k and γ of the Si substrate ($c \ll b$). On the other hand we can not say the same think about α . One can easily see that: $\alpha_{\text{Si}} \ll \alpha_{\text{Cu}}, \alpha_{\text{Al}}, \alpha_{\text{Ag}}, \alpha_{\text{Au}}$.

The absorption coefficient is an essential parameter of the $A(r, z, t)$. In order to describe the global situation (for having a unique heat equation) we propose the following heat absorption coefficient:

$$\alpha_{total} = \alpha_{\text{Si}} + (1/2) \cdot [\alpha_{\text{thin film}} + \alpha_{\text{thin film}} \cdot \text{Tanh}(\alpha_0 \cdot z)] \quad (4)$$

For example:

$$\alpha_{total} = \alpha_{\text{Si}} + (1/2) \cdot [\alpha_{\text{Al}} + \alpha_{\text{Al}} \cdot \text{Tanh}(\alpha_0 \cdot z)] \quad (5)$$

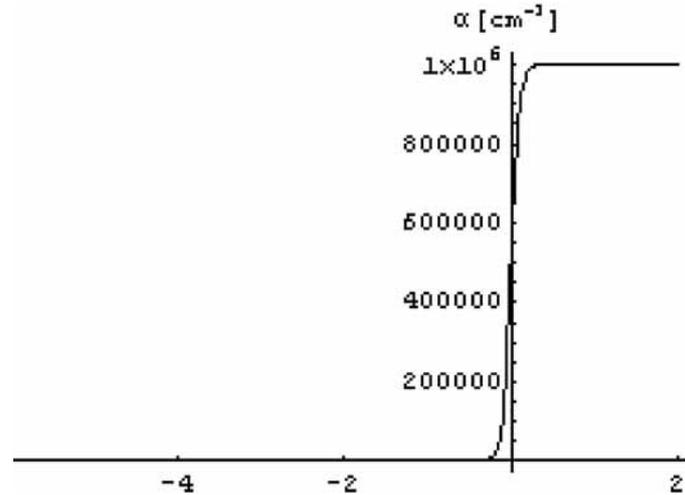


Fig. 1 – The absorption coefficient at the Si-Al interface when $\alpha_0 = 10$ versus the z -distance (along the beam propagation) in μm . The length of the interface is about $0.6 \mu\text{m}$.

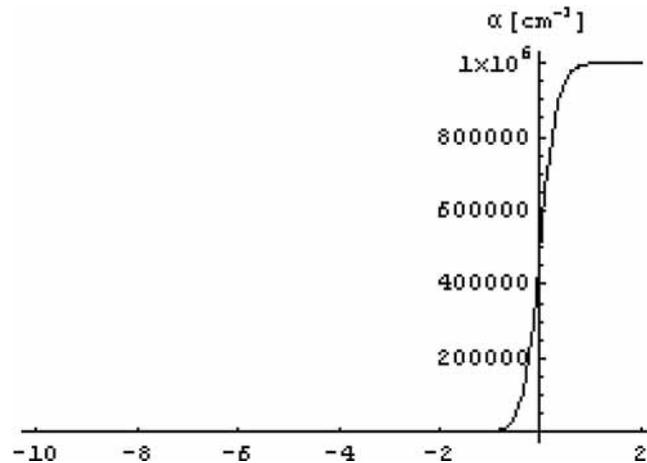


Fig. 2 – The absorption coefficient at the Si-Al interface when $\alpha_0 = 3$ versus the z -distance (along beam propagation) in μm . The length of the interface is about $2 \mu\text{m}$.

One can see that the parameter α_0 gives us a typical measure of the interface substrate-thin-film. We call this approximation a semi-classical approach; because the parameter α_0 can easily describes the absorption at the interface; which is of a quantum nature. In conclusion we will treat a solid consisting from a substrate (let say Si) and a thin film (let say Al) like a unique solid with γ and K given by the substrate and α given by the formula (5).

4. RESULTS AND DISCUSSION

We have:

$$A(r, z, t) = \alpha \cdot I_0 \cdot e^{-\alpha \cdot z} \cdot e^{-2r^2/w^2} (h(t) - h(t - t_0)). \quad (6)$$

Here I_0 is the maximum intensity of the laser beam; $w = 7\text{mm}$ is the width of the free electron laser beam (which is supposed to be Gaussian (TEM₀₀)); h is the Heaviside step function; t is the time and t_0 is the length of the laser pulse.

Using the integral transform method the solution of the heat equation is [16–19]:

$$T(r, z, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left[f(\mu_i, \lambda_j) \cdot (\mu_i^2 + \lambda_j^2)^{-1} \cdot \left(1 - e^{-\beta_{ij}^2 \cdot t} - \left(1 - e^{-\beta_{ij}^2 \cdot (t-t_0)} \right) h(t-t_0) \right) \right] \times K_r(\mu_i, r) \cdot K_z(\lambda_j, z) \quad (7)$$

where: $\beta_{ij}^2 = \gamma^2 (\mu_i^2 + \lambda_j^2)$.

The functions: $K_r(\mu_i, r)$ and $K_z(\lambda_j, z)$ are the eigenfunctions of the integral operators applied to the heat equation and the variables μ_i and λ_j are the eigenvalues corresponding to the same operators:

$$K_r(\mu_i, r) = \cos(\lambda_j \cdot z) + \frac{h}{k \cdot \lambda_j} \sin(\lambda_j \cdot z) \quad \text{and} \quad K_z(\lambda_j, z) = J_0(\mu_i \cdot r).$$

The term that contains the absorption coefficient is:

- the coefficients C_i and C_j are the normalizing coefficients [16, 17]:

$$f(\mu_i, \lambda_j) = \frac{\alpha \cdot I_0}{K \cdot C_i \cdot C_j} \int_b^c e^{-\alpha \cdot z} K_z(z, \lambda_j) dz \int_0^a r e^{-2r^2/w_0^2} K_r(r, \mu_i) \cdot dr \quad (8)$$

$$C_i = \int_0^a r \cdot K_r^2(r, \mu_i) dr = \frac{a^2}{\mu_i^2} \left(\frac{h^2}{k^2} + \mu_i^2 \right) \cdot J_0^2(\mu_i a) \quad \text{and} \quad C_j = \int_b^c K_z^2(z, \lambda_j) dz.$$

The eigenvalues μ_i and λ_j can be obtained using the boundary condition from equations (2) [16, 17]:

$$2 \cdot \cot(\lambda_j b) = \frac{\lambda_j k}{h} - \frac{h}{k \lambda_j}, \quad \frac{h}{k} J_0(\mu_i \cdot a) - \mu_i J_1(\mu_i a) = 0.$$

We consider a sample with the substrate with: $b = -10\text{ mm} \leq z \leq 0$ and the thin film: $0 \leq z \leq 2\text{ }\mu\text{m}$. The radius of the sample is $a = 10\text{ mm}$. We consider that

the solid is irradiated with a free electron laser with 20 ns, the mode TEM_{00} and 20 kW power. In Fig. 3 the thermal field at the interface ($z = 0$) is presented considering that the sample is formed only on the substrate (without considering any thin film). The plot presents the thermal field in the first 20 ns. The same thermal field is presented in Fig. 4, but for the first 10^{-5} s. One can notice that the maximum of the thermal field is obtained in the center of the sample ($r = 0$), where laser beam has it's maximum intensity. We can also observe that after 10^{-5} s the cooling process starts. In Fig. 5 we present the thermal field corresponding to a system having the absorption coefficient given in Fig. 1; at the interface ($z = 0$). In Fig. 6 is present the thermal field corresponding to a system having the absorption coefficient given in Fig. 2.

One can notice that: (i) the thermal field depends strongly on the absorption coefficient of the thin film and (ii) the length of the interface, at least in the range: $0.1\text{--}10\ \mu\text{m}$, does not play an important role in the thermal fields.

Fig. 7 presents the thermal field at the surface ($z = -10\ \text{mm}$ and $r = 0$), for the absorption coefficient presented in Fig. 1. We can also notice an increase of about 1 K due to the presents of the thin film. Thus we have developed a model which

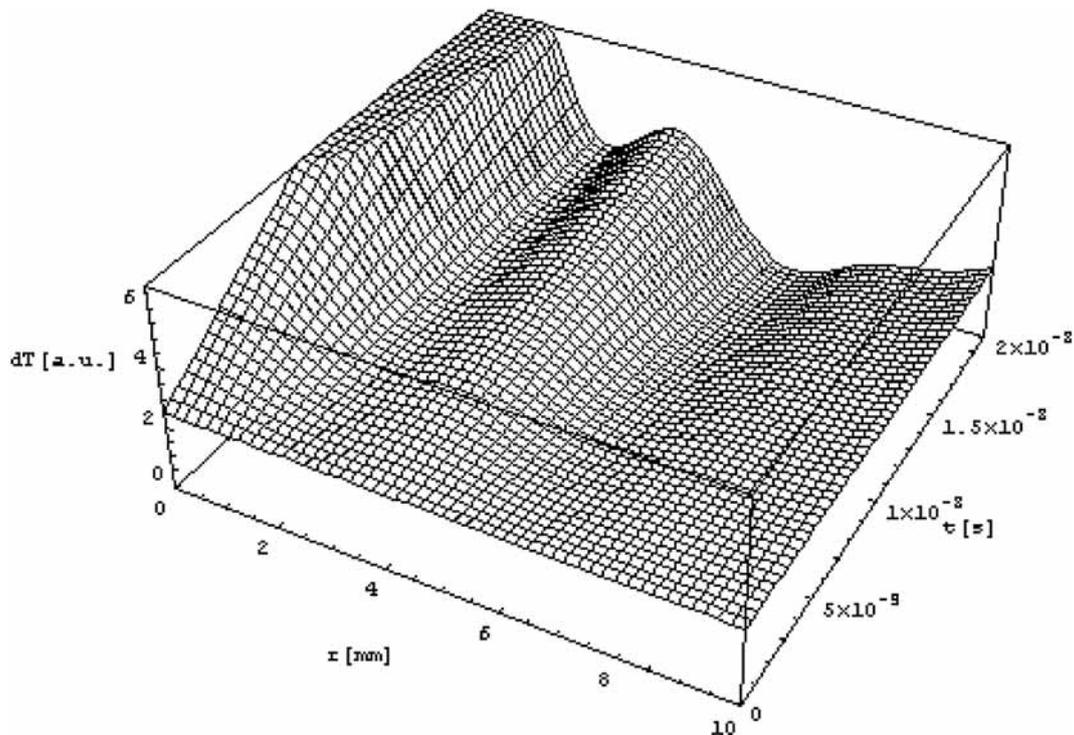


Fig. 3 – The thermal field at the interface considering that the sample is formed only on the substrate (without considering any thin film), for the first 20 ns.

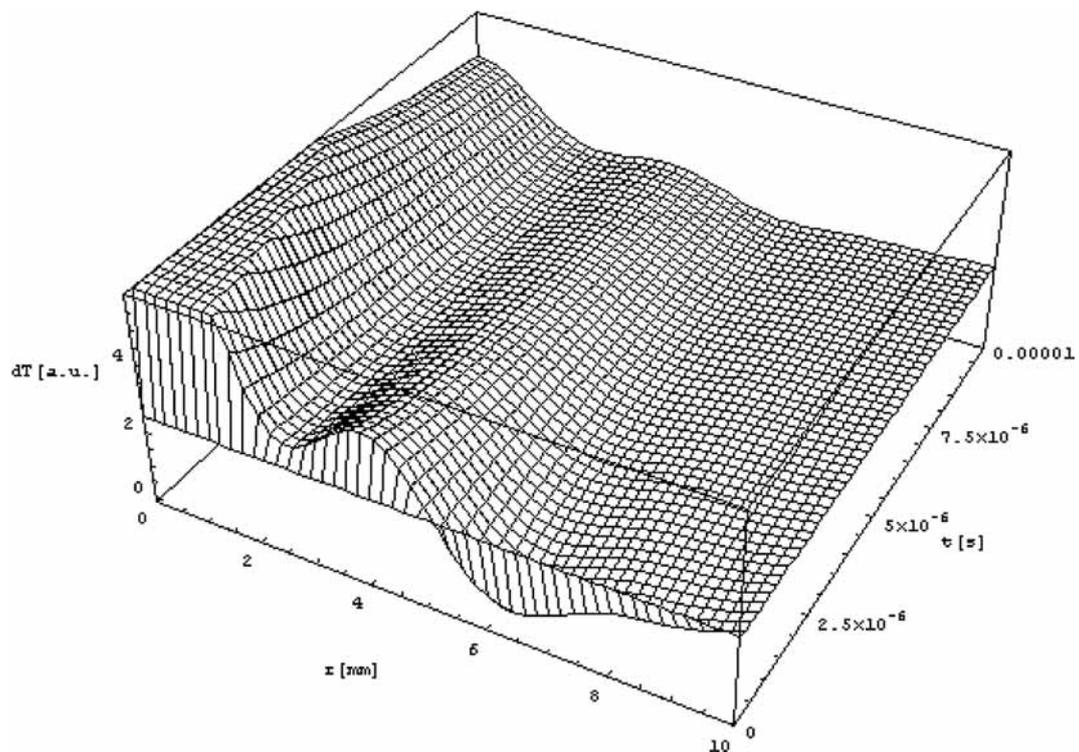


Fig. 4 – The thermal field at the interface ($z = 0$) considering that the sample is formed only on the substrate (without considering any thin film), for the first 10^{-5} s.

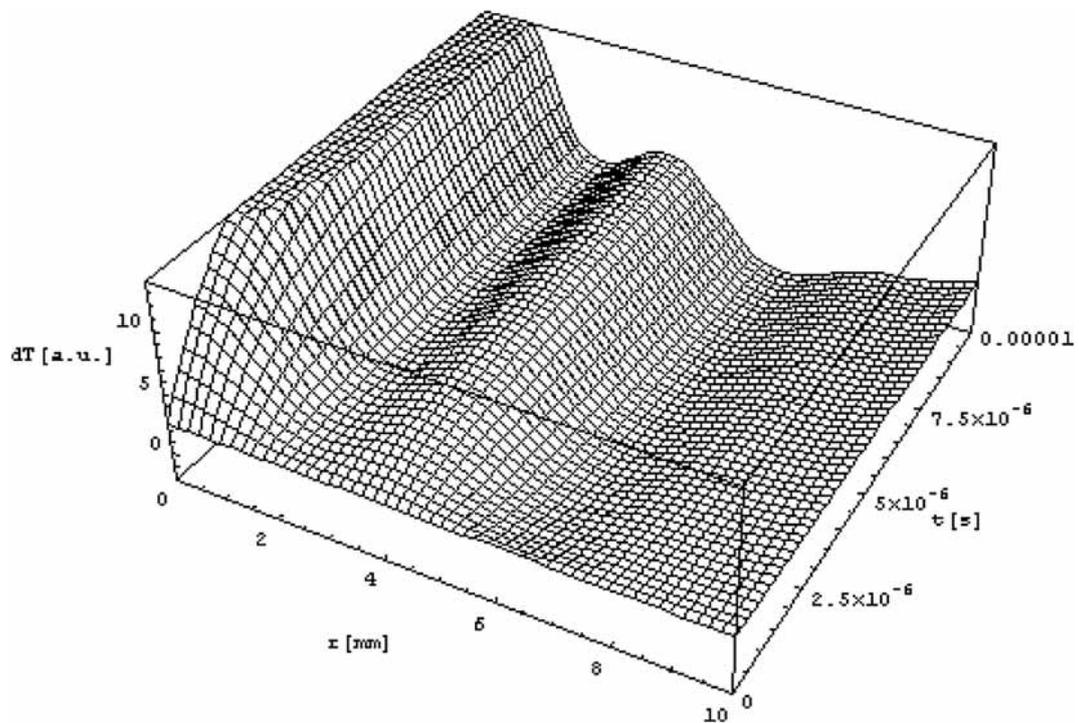


Fig. 5 – The thermal field corresponding to a system having the absorption coefficient given in Fig. 1; at the interface ($z = 0$).

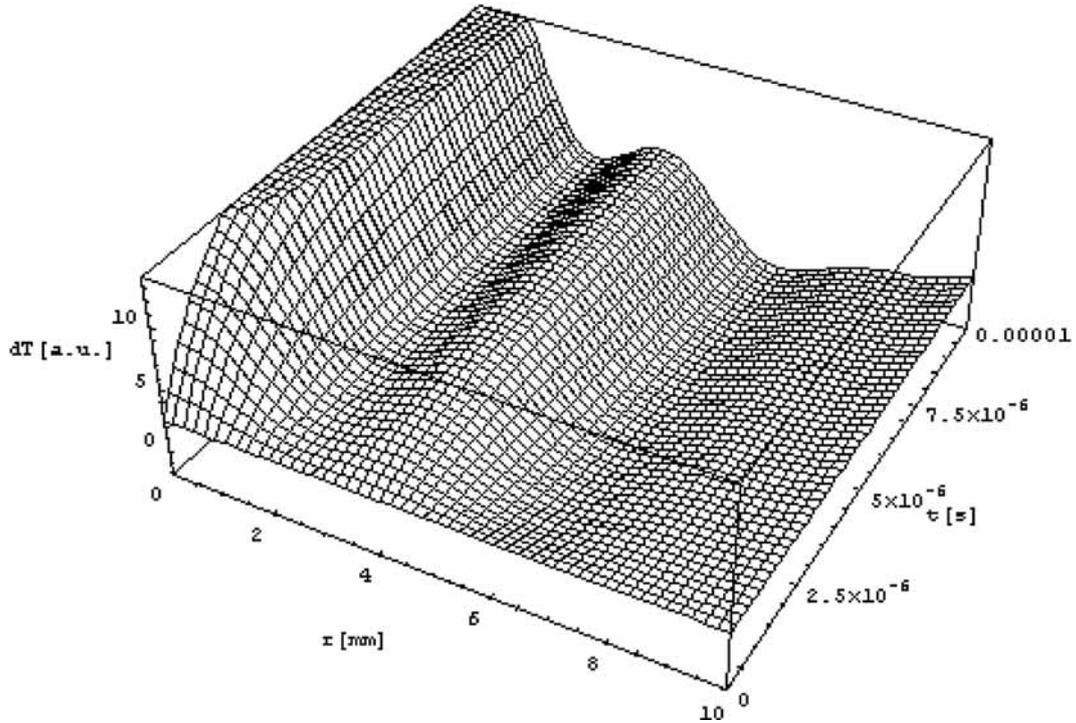


Fig. 6 – The thermal field corresponding to a system having the absorption coefficient given in Fig. 2; at the interface ($z = 0$).

can be applied to systems which have substrates and thin films with thermal parameters of the same order of magnitude.

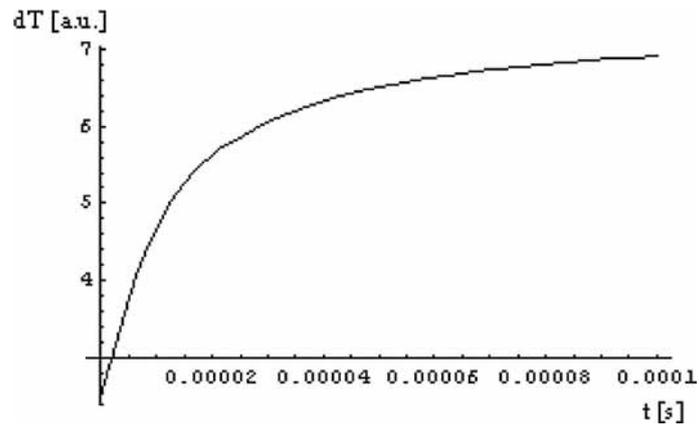


Fig. 7 – The thermal field versus time (in seconds) at the surface ($z = -10$ mm and $r = 0$), for the absorption coefficient presented in Fig. 1.

5. OUTLOOK

In this section we discuss the differences (from an experimental point of view) between classical laser calorimetry and free electron laser calorimetry. We want to answer to the fundamental question: Is it realistic to realize free electron laser calorimetry? The problem has a simple answer: the difference (between the two kind of calorimetries) exists because of the huge intensity provided by free electron lasers in comparison with “atomic” lasers. This observation leads us to the second question. The problem is how to avoid the thermal runaway. We consider three ways.

First of all is to consider a huge heat transfer coefficient in order to take a part of the heat. This can be done, for example, by using a cooling fluid around the sample.

Another possibility is to use just one ultra-short laser-pulse, because, as we have seen in our simulations: the shorter the pulse time the lower the temperature is.

The third possibility is to consider solid samples here, for example, that the linear absorption coefficient is zero (due to the quantum mechanical selection rules). In this case we have high photon absorption coefficients, (which present very low cross section interaction) and in consequence very low temperatures.

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