

New analytical heat transfer model for weak laser-crystalline solids interaction

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We propose a coherent mathematical model for laser processing of crystalline solids when the solid's temperature variation is small (up to 100 K-300 K). In fact, we treat the heat equations for two major cases fulfilling our condition: *i*) the sample's absorption coefficient is very small (e.g. ZnSe, GaAs.); and/or *ii*) the laser intensity is not very high. The condition of small temperature variations has two advantages: validates the assumption on thermal independence for optical and thermal parameters (such as thermal diffusivity, thermal conductivity, heat transfer coefficient and absorption coefficient) and the possibility to make use of the linear heat absorption coefficients hypothesis. We present a number of three theorems in order to help the experimentalists in their work in the field of thermal effects in laser-matter interaction.

(Received September 10, 2012; Accepted September 30, 2012)

Keywords: Laser processing, Heat equation, Integral transform

1. Introduction

In order to solve very "exotic" forms of the heat equation, we use the integral transform technique, which have been developing in the early '60s (Koshlyakov N. S. *et al.*, 1964). Our models are more powerful than Green function method, Fourier series or perturbation methods. We are searching analytically and semi-analytically solutions of various heat equations. Our semi-analytically solutions become analytically if we consider the first 10 eigen-values for each spatial coordinate. The computer simulations show that using only the first 10 eigen-values, the solutions are so quickly convergent that the absolute error in determining the temperature field is about 10^{-2} K. We discuss five important theorems concerning the solutions of the heat equations for different situations in laser processing. The first theorem is due to interaction of a laser beam that has like intensity a combination of transverse modes TEM_{mn} , and a homogenous solid target. The second theorem is a generalization of the first theorem, with the specification that the laser beam is moving. Theorem 3 is a powerful one, including quantum effects in classical heat equation such as the absorption of one, two, three and four photons. In this way, we obtain a semi-classical heat equation. We believe that our mathematical model could be of great help to people working in laser processing area.

It is very easy to find out solutions to a heat equation considering the very simple models of interaction. As long as one faces realistic situations involving more complicated interaction models, the heat equations become more and more difficult to be solved [1, 2, 3].

We first discuss two approximations used for solving different heat equations [4, 5, 6, 7]. The first one treats the supposition of linearly approximation of the boundary conditions. If the flux across the surface is proportional to the temperature difference between the

surface and the surrounding medium, so that it is given by $h(T - T_0)$ where T is the temperature of the sample, T_0 is the temperature of the medium and h is the transfer coefficient, the boundary condition is $K(\partial T / \partial n) + h(T - T_0) = 0$, where n is the normal to the surface and K is the sample thermal conductivity. If $T - T_0$ is not large (which is the basic assumption of the present article), one can apply the linear heat transfer approximation: $h_{rad} = 4\sigma ET_0^3$ where σ is the Stefan-Boltzmann constant and E is the emissivity of the surface.

From experimental point of view the heat transfer coefficient should also contain the convection contribution, which in many cases becomes dominant over the radiation loses. For the convection heat transfer we can use the linear approximation. In this situation, both effects can be considered by an approximate value of a linear heat transfer coefficient: $h = h_{rad} + h_{conv}$.

The second approximation refers to the thermal independence of the optical and thermal parameters included in the heat equations. This is a very important assumption; if we consider the thermal dependence of the mentioned parameters, we are force to use numerical models.

2. Theorem No. 1

The heat equation in the case of laser irradiation of a homogeneous solid sample (cylinder with height a and radius b) is:

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

(Where: γ is the thermal diffusivity, k is thermal conductivity, and $A(r, \phi, z, t)$ is the heat rate variation per unit volume and time). The boundary conditions are:

$$\begin{aligned} K \left. \frac{\partial T(r, \phi, z, t)}{\partial r} \right|_{r=b} + hT(b, \phi, z, t) &= 0 \\ K \left. \frac{\partial T(r, \phi, z, t)}{\partial r} \right|_{z=0} - hT(r, \phi, 0, t) &= 0 \\ K \left. \frac{\partial T(r, \phi, z, t)}{\partial r} \right|_{z=a} + hT(r, \phi, a, t) &= 0 \end{aligned} \quad (2)$$

The ‘‘periodicity’’ conditions are in this case as follows:

$$T(r, 0, z, t) = T(r, 2\pi, z, t). \quad (3)$$

The temperature T is a function of (r, ϕ, z, t) and is defined as the temperature variation. We have therefore $T(r, \phi, z, 0) = 0$.

If we consider the case of a continuous-wave (cw) CO₂ laser source operated in the transversal modes $\{mn\}$, we have the following solution of Eq. (2):

$$\begin{aligned} T(r, \phi, z, t) &= \sum_{m,n} \sum_{i=1}^{\infty} \sum_{l=0}^{\infty} \sum_{j=1}^{\infty} \hat{f}_{2l}(\mu_{il}, \lambda_j, l) \cdot g(\mu_{il}, \lambda_j, t) \times K_r(\mu_{il}, r) \times K_\phi(2l, \phi) \times K_z(\lambda_j, z) + \\ &\sum_{m,n} \sum_{i=1}^{\infty} \sum_{l=0}^{\infty} \sum_{j=1}^{\infty} \hat{f}_{2l-1}(\mu_{il}, \lambda_j, l) \cdot g(\mu_{il}, \lambda_j, t) \times K_r(\mu_{il}, r) \times K_\phi(2l-1, \phi) \times K_z(\lambda_j, z) \end{aligned} \quad (4)$$

Here:

$$\begin{aligned} \hat{f}_{2l}(\mu_{il}, \lambda_j, l) &= \frac{1}{k\pi C_{il} C_j} \int_0^a \alpha \cdot e^{-\alpha z} \times K_z(\lambda_j, z) dz \times \\ &\int_0^b \int_0^{2\pi} I_{mn}(r, \phi) \cdot r \times K_r(\mu_{il}, r) \times K_\phi(2l, \phi) dr d\phi \end{aligned} \quad (5)$$

And

$$\begin{aligned} \hat{f}_{2l-1}(\mu_{il}, \lambda_j, l) &= \frac{1}{k\pi C_{il} C_j} \int_0^a \alpha \cdot e^{-\alpha z} \times K_z(\lambda_j, z) dz \times \\ &\int_0^b \int_0^{2\pi} I_{mn}(r, \phi) \cdot r \times K_r(\mu_{il}, r) \times K_\phi(2l-1, \phi) dr d\phi \end{aligned} \quad (6)$$

Where

$$\begin{aligned} I_{mn}(x, y) &= I_{0mn} \left[H_m \left(\frac{\sqrt{2}x}{w} \right) H_n \left(\frac{\sqrt{2}y}{w} \right) \times \exp \left[- \left(\frac{x^2 + y^2}{w^2} \right) \right] \right]^2 \\ g(\mu_{il}, \lambda_j, t) &= 1 / (\mu_{il}^2 + \lambda_j^2) [1 - e^{-\beta_{ij}^2 t} - (1 - e^{-\beta_{ij}^2 (t-t_0)}) h(t-t_0)] \end{aligned} \quad (7)$$

Here $\beta_{ij}^2 = \gamma(\mu_{il}^2 + \lambda_j^2)$, $h(t-t_0)$ is the Heaviside function and t_0 the exposure time. The functions $K_r(\mu_{il}, r)$, $K_\phi(2l, \phi)$, $K_\phi(2l-1, \phi)$ and $K_z(\lambda_j, z)$ are eigen-functions corresponding to the eigen-values μ_{il} , $2l$, $2l-1$, λ_j . We have $K_r(\mu_{il}, r) = J_1(\mu_{il} \cdot r)$, $K_\phi(2l, \phi) = \cos(l\phi)$, $K_\phi(2l-1, \phi) = \sin(l\phi)$ and

$$K_z(\lambda_j, z) = \cos(\lambda_j \cdot z) + (h/k\lambda_j) \cdot \sin(\lambda_j z).$$

Proof of theorem No. 1:

The heat equation inside cylindrical samples (Eq. (1)), was solved using the integral operators’ method. To eliminate differentiation with respect to ϕ , we set $D_\phi = \partial^2 T / \partial \phi^2$.

The auxiliary function $\bar{K}_\phi(\gamma, \phi) = (1/\pi) K_\phi(\gamma, \phi)$ must satisfy the equation $(\partial^2 \bar{K}_\phi / \partial \phi^2) + l^2 \bar{K}_\phi = 0$ and the periodicity condition $\bar{K}_\phi|_{\phi=0} = \bar{K}_\phi|_{\phi=2\pi}$.

The solution of these equations is

$$\bar{K}_\phi(\gamma, \phi) = \begin{cases} \frac{1}{\pi} \cos(l\phi) & \text{for } \gamma = 2l \\ \frac{1}{\pi} \sin(l\phi) & \text{for } \gamma = 2l-1 \end{cases}.$$

Applying $\bar{K}_\phi(\gamma, \phi)$, Eq. (1) becomes

$$\frac{\partial^2 \bar{T}}{\partial r^2} + \frac{1}{r} \frac{\partial \bar{T}}{\partial r} + \frac{\partial^2 \bar{T}}{\partial z^2} - \frac{l^2}{r^2} \bar{T} - \frac{1}{\gamma} \frac{\partial \bar{T}}{\partial t} = -\frac{\bar{A}(r, l, z, t)}{k} \quad (8)$$

Where:

$$\bar{T}(r, \gamma, z, t) = \bar{T}(r, l, z, t) = \int_0^{2\pi} T(r, \phi, z, t) \bar{K}_\phi(l, \phi) d\phi$$

$$\text{and } \gamma = \begin{cases} 2l \\ 2l-1 \end{cases}$$

To eliminate differentiation with respect to r , we set

$$D_r \bar{T} = \frac{\partial^2 \bar{T}}{\partial r^2} + \frac{1}{r} \frac{\partial \bar{T}}{\partial r} - \frac{l^2}{r^2} \bar{T}$$

The auxiliary function $\tilde{K}_r(\mu_{il}, r) = K_r(\mu_{il}, r) \times (1/C_{il}) r$ must satisfy the equation:

$$\frac{\partial}{\partial r} \left(r \frac{\partial \tilde{K}_r}{\partial r} \right) - \frac{l^2}{r} \tilde{K}_r + \mu^2 r \tilde{K}_r = 0$$

and the boundary condition

$$\tilde{K}_r \Big|_{r=0} < \infty, \quad \left[k \frac{\partial \tilde{K}_r}{\partial r} + h \tilde{K}_r \right]_{r=b} = 0.$$

The solution is $\tilde{K}_r(\mu_{il}, r) = J_l(\mu_{il} r) (1/C_{il}) r$

Where

$$C_{il} = \int_0^b r [J_l(\mu_{il} r)]^2 dr = 1/2 \mu_{il}^2 [b^2 (h/k)^2 + b^2 \mu_{il}^2 - l^2] J_l^2(\mu_{il} b)$$

and μ_{il} is given by $\mu_{il} J_l'(\mu_{il} b) + h J_l(\mu_{il} b) = 0$.

Applying $\bar{K}_r(\mu_{il}, r)$ Eq. (8) becomes

$$-\mu_{il} \tilde{T} + \frac{\partial^2 \tilde{T}}{\partial z^2} - \frac{1}{\gamma} \frac{\partial \tilde{T}}{\partial t} = -\frac{\tilde{A}(\mu_{il}, z, t)}{k} \quad (9)$$

where $\tilde{T}(\mu_{il}, z, t) = \frac{1}{C_{il}} \int_0^b \bar{T}(r, l, z, t) r J_l(\mu_{il} r) dr$.

To eliminate the differentiation with respect to z , we set

$$D_z \tilde{T} = \frac{\partial^2 \tilde{T}}{\partial z^2}. \quad \text{The function}$$

$\hat{K}_z(\lambda_j, z) = (1/C_j) K_z(\lambda_j, z)$ must satisfy

$\partial^2 \hat{K}_z / \partial z^2 + \lambda \hat{K}_z = 0$ and the boundary conditions

$$\left[k(\partial \hat{K}_z / \partial z) - h \hat{K}_z \right]_{z=0} = 0,$$

$$\left[k(\partial \hat{K}_z / \partial z) + h \hat{K}_z \right]_{z=a} = 0.$$

The function is

$$\hat{K}_z = (1/C_j) (\cos(\lambda_j z) + (h/k\lambda_j) \sin(\lambda_j z))$$

where $C_j = \int_0^a \hat{K}_z^2(\lambda_j, z) dz$ and λ_j is given by

$$2 \cot(\lambda_j a) = (\lambda_j k/h) - (h/\lambda_j k).$$

Applying $\hat{K}_z(\lambda_j, z)$ Eq. (9) becomes:

$$\mu_{il} \hat{T} + \lambda_j \hat{T} + \frac{1}{\gamma} \frac{\partial \hat{T}}{\partial t} = \frac{\hat{A}(\mu_{il}, \lambda_j, t)}{k} \quad (10)$$

Using the direct and inversion Laplace transform technique one can solve Eq. (10) and obtain the solutions of the first theorem. An application to the theorem No. 1 is shown in Fig. 1.

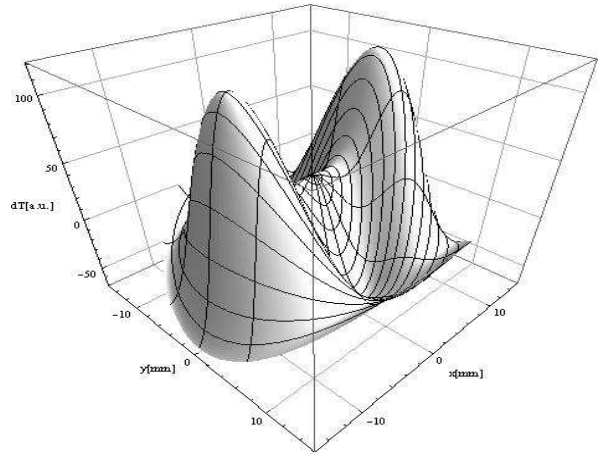


Fig. 1 The thermal field generated in bulk Cu by a cw CO₂ laser source operating in TEM₀₃ at 10 W, stationary ($v = 0$) on the sample surface, irradiation time 10 s.

3. Theorem No. 2

We next consider the case of a laser beam in motion on the Cu sample surface with a velocity v . The components of the velocity along the two axes are v_x and v_y , respectively. A new reference system with the coordinates $x = x_0 + v_x \cdot t$ and $y = y_0 + v_y \cdot t$ is introduced and adapted correspondingly to the source term.

We perform calculations for $v_x = 10$ mm/s, $v_y = 0$, $t = 10$ s (Fig. 2) and $t = 20$ s (Fig. 3). As in the case presented in Fig. 1, the cw CO₂ laser beam was operating in the TEM₀₃ transversal mode at an output power of 10 W.

By comparing Fig. 1 to Fig. 2 and Fig. 3, we first notice that the two temperature maxima are present in all cases. The main difference is due to the depth of the

minimum between the two peaks, which is decreasing from Fig. 1 to Fig. 3. The differences between the minimum and maximum temperatures are diminishing and the plateau between the two maxima moves to higher temperatures. This observation is congruent with a uniform heating of the sample as an effect of the laser beam movement. This effect is more pronounced in the case of a higher velocity of the laser beam.

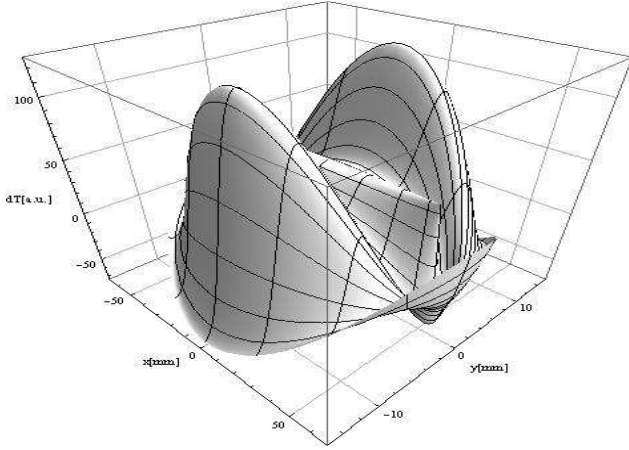
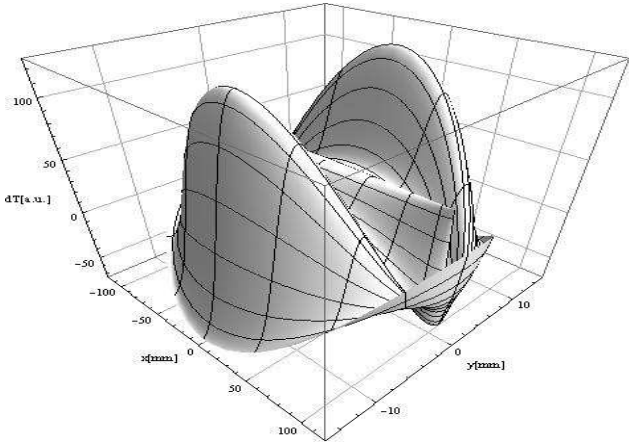


Fig. 2 Thermal field generated in bulk Cu by a cw CO₂ laser source operating in TEM₀₃ at 10 W scanning the sample surface with $v_x = 10$ mm/s irradiation time 10 s



$$A(r, z, t) = (\alpha_1 \cdot I_{00}(r, z) + \alpha_2 I_{00}^2(r, z) + \alpha_3 I_{00}^3 + \alpha_4 I_{00}^4 + r_s \delta(z)) \cdot (h(t) - h(t - t_0)) \quad (13)$$

Where: t_0 is the pulse duration, $h(t)$ is the step function and r_s is the surface absorption coefficient.

Fig. 3 Thermal field generated in bulk Cu by a cw CO₂ laser source operating in TEM₀₃ at 10 W scanning the sample surface with $v_x = 10$ mm/s irradiation time 20 s.

The proof of the second theorem is identical with the proof of the first theorem with the mention that we have to make the changes: $x_0 \rightarrow x$ and $y_0 \rightarrow y$.

4. Theorem No. 3

The macroscopic heat equation is employed to investigate the temperature field in a (InSb) semiconductor exposed to a CO₂ laser with a Gaussian spatial profile and a rectangular nanosecond pulse. The sample is supposed to be homogeneous and therefore, there is no angular dependence on the temperature variation. The equation describing the heat diffusion inside a cylindrical solid sample irradiated by a laser beam centred to the probe is:

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} - \frac{1}{\gamma} \frac{\partial T}{\partial t} = -\frac{A(r, \varphi, z, t)}{k} \quad (11)$$

In the presence of one-, two-, three- and four- photon-absorption, described by coefficient α_i , the change in the light intensity as it passes through the sample is:

$$\frac{dI}{dx} = -\alpha_1 I - \alpha_2 I^2 - \alpha_3 I^3 - \alpha_4 I^4 \quad (12)$$

In order to consider the multi-photon absorption, the heat rate per unit volume and time is calculate using the Beer's law:

$$T_{\alpha_1, \alpha_2, \alpha_3, \alpha_4}(r, z, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left[\frac{1}{\mu_i^2 + \lambda_j^2} \cdot f_{\alpha_1, \alpha_2, \alpha_3, \alpha_4}(\mu_i, \lambda_j) \cdot (1 - e^{-\theta_{ij}^2 t} - (1 - e^{-\theta_{ij}^2(t-t_0)}) \cdot h(t-t_0)) \right] \times \\ \times K_r(\mu_i, r) \cdot K_z(\lambda_j, z) \quad (14)$$

where $\theta_{ij}^2 = \gamma(\mu_i^2 + \lambda_j^2)$ and

$$f_{\alpha_1, \alpha_2, \alpha_3, \alpha_4}(\mu_i, \lambda_j) = \frac{1}{k C_i C_j} \int_0^a \int_0^b [(\alpha_1 I_{00} + \alpha_2 I_{00}^2(r, z) + \alpha_3 I_{00}^3 + \alpha_4 I_{00}^4 + r_s \delta(z)) r \cdot \\ \cdot K_r(\mu_i, r) \cdot K_z(\lambda_j, z)] dr dz \quad (15)$$

C_i and C_j are normalizing coefficients. The eigen-values μ_i and λ_j correspond to the eigen-functions $K_r(r, \mu_i)$ and $K_z(z, \lambda_j)$. The integral operators corresponding to the eigen-functions $K_r(r, \mu_i) = J_0(\mu_i \cdot r)$ and

$K_z(z, \lambda_j) = \cos(\lambda_j z) + \frac{h}{\lambda_j k} \sin(\lambda_j \cdot z)$ are normalized by the following coefficients:

$$C_i = \int_0^b r K_r^2(r, \mu_i) dr = \frac{b^2}{2\mu_i^2} \left(\frac{h^2}{k^2} + \mu_i^2 \right) J_0^2(\mu_i b) \quad (16)$$

And

$$C_j = \int_0^a K_z^2(z, \lambda_j) dz = \frac{1}{4\lambda_j^3} \left(2\frac{h}{k}\lambda_j + 2a\frac{h^2}{k^2} \lambda_j + 2a\lambda_j^3 - 2\frac{h}{k}\lambda_j \cos[2a\lambda_j] - \right. \\ \left. - \frac{h^2}{k^2} \sin[2a\lambda_j] + \lambda_j^2 \sin[2a\lambda_j] \right) \quad (17)$$

The eigen-values μ_i and λ_j are determined from the boundary conditions.

5. Results and discussion regarding theorem no. 3

In the previous section, the heat diffusion equation was analytically solved in order to determine the temperature field inside a semiconductor sample. One cylindrical InSb sample of radius: $b = 10$ mm and thickness $a = 4$ mm, was considered. The sample was supposed to be irradiating by a 5 ms TEM₀₀ CO₂ laser beam of 100 W power and 2 mm width. The InSb sample's characteristics are mass density $\rho = 5.78$ g/cm³ thermal conductivity $k = 16$ W/mK specific heat $c = 0.144$ J/g °C absorption coefficient $\alpha = 0.64$ mm⁻¹ two-photon absorption coefficient $\beta = 15$ cmMW⁻¹. A typical temperature distribution versus time and radial coordinate, neglecting the two absorption coefficient ($\beta = 0$), for a 5 ms TEM₀₀ CO₂ laser beam is shown in Fig. 4. The temperature distribution reaches its maximum in the sample centre, in the point where power density has its maximum. Our simulation shows that if we consider $\beta = 15$ cmMW⁻¹ the temperature field increases with 3.34% in respect to the maximum temperature field of the $\beta = 0$ case (Fig. 4).

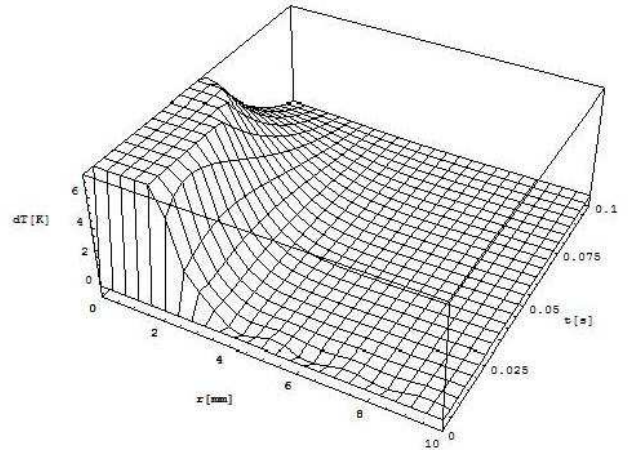


Fig. 4 Computed temperature field inside InSb probe exposed for 5 ms to a 100 W TEM₀₀ CO₂ laser beam

6. General discussions

There are many methods for measuring the thermal fields in laser-matter interaction but most of them require a complex mathematical apparatus as well very complicated experimental setup.

Our paper presents a direct and powerful mathematical theory to compute the thermal field. The solving procedure is base on applying the integral

transform technique, which was developed in 1960, by the Russian school of theoretical physics [1].

The comparison with data from literature [2, 3] is in good agreement with our model [4, 5, 6, 7]. We conclude that our analysis is quite general, but its application fails as soon as the material is melted and vaporized under irradiation.

At the end of our conclusions, we should mention that there are other models competitive with our model. These models are in general more complicated, but may be used in parallel with our model in order to extract more information [8].

For example, in reference [8] it is avoided the Fourier differential heat equation and it is used the Duhamel's principle which leads to a convolution, integrated analytically by using a Taylor series approximation.

We conclude that our model [9, 10, 11, 12] is direct and powerful enough to give rapidly and correctly the first information on the temperature distribution for laser-material interaction.

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