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The generalized heat equation for laser- crystalline solid interaction

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The present paper is an approach to solve the semi-classical heat equation for the laser-solid interaction. The term "semi-classical heat equation" is due to the introduction in the source term of quantum phenomena such as absorption of n_{ph} photon. Consequently we consider that the interaction is done via n-photon absorption, where n_{ph} can vary from1 to $n_{max.}$ The solid is supposed to have a layered structure, each layer having a linear form for the thermal conductivity. In our model the laser is acting in few decoupled Hermite-Gauss modes. For solving the heat equation, the powerful method of integral transforms was used. In fact we generalized our previous theorem [Oane. M, S. L. Tsao, F. Scarlat, Temperature field distribution in multi-layered solid media heated with multi-modes laser beam, Optics Laser Technol 2006, in press].

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1. Introduction

In the last century a new form of light, laser light, has provided important contribution 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. The theory of heat conduction was well studied long time age [2-9]. For describing this interaction the classical heat equation was used in a lot of applications. Apart of some criticism [10], the heat equation still remains a powerful tool in describing the thermal effects in laser-solid interaction [11-13]. The heat equation can be used for describing both: interaction with homogeneous [14-17] and non-homogeneous solids [18-20]. A special attention was given to multi-layered samples and thin films [21-33].

The purpose of this paper is to discuss some solutions to the basic heat equation. It is well know that solutions to the heat equation can only be obtained in simple analytical form only when one is prepared to make a variety of assumptions regarding the spatial and temporal dependence on the heat source and on the geometry of the sample. As the description of these boundary conditions becomes more and more rigorous in terms of the actual spatial and temporal dependence on the heat source, and on the geometry of the sample, analytical and semi-analytical solutions of the heat equation can no longer be obtained. The main goal of the present paper is to present a very complicate form of the heat source, the sample description and the interaction between them in order to still get a semi-analytical solution.

In the present paper, we consider that the solid sample is multilayered, each layer having a linear thermal conductivity. The laser beam is supposed to act in few decoupled Hermite-Gauss modes. The laser-solid interaction is approached as general as possible, considering the n-photon absorption, where n_{ph} can vary from1 to $n_{max.}$ For solving the heat equation the integral transform method was applied [14-17]. Our approached relied on the consideration that the solid target has the thermal parameters almost constant during the heating, otherwise semi-analytical solutions can not be obtained. Consequently the present model is excellent for laser windows, which show low absorption coefficients (like for example ZnSe, GaAs, etc.).

On the other hand the multi-photon absorption processes in crystalline solids have been the subject of extensive theoretical and experimental investigations since the advent of the laser over four decades ago. The interest in the multi-photon absorption has been stimulated by the importance of nonlinear absorption in high-power laser technology as well as by its fundamental role in solid-state physics.

2. The laser-solid interaction

For describing the interaction between laser beam and crystalline solid, the most general form of interaction was considered. So let's consider the n-photon absorption phenomena, where n_{ph} can vary from 1 to $n_{max.}$ The multi-photon absorption can be described by the Beer-Lambert law: $\frac{dI}{dx} = -\sum_{n_{ph}} \alpha_{n_{ph}} I^{n_{ph}}$ where $\alpha_{n_{ph}}$ is the n-photon absorption coefficient, I is the light flux and x is the propagation direction. We have: $\alpha_{n_{ph}} = 2W_{n_{ph}} n\hbar\omega / I^{n_{ph}}$ where I is the incident radiation intensity and the factor 2 accounts for electron-spin degeneracy. The n-photon transition probability $W_{n_{ph}}$ is given by the Goppert-Mayer n th-order time-dependent perturbation theory The probability of a direct electronic transition from an initial valence band υ to a final conduction band *c*, accompanied by the simultaneous absorption of n photons, each of frequency ω is expressed by:

$$W_{n_{ph}} = \frac{2\cdot\pi}{\hbar}\int\left|\sum_m\sum_l\cdots\sum_j\sum_i \frac{\langle\psi_c|H|\psi_m\rangle\langle\psi_m|H|\psi_l\rangle}{[E_m-E_l-(n-1)\hbar\omega]}\cdots\frac{\langle\psi_j|H|\psi_i\rangle}{(E_j-E_i-2\hbar\omega)}\frac{\langle\psi_i|H|\psi_\upsilon\rangle}{(E_i-E_\upsilon-\hbar\omega)}\right|^2 \times\delta[E_c(\vec{k})-E_\upsilon(\vec{k})-n\hbar\omega]\frac{d^3\vec{k}}{(2\pi)^3}$$

where: $\psi_i, \psi_j \ldots$ are the Bloch functions of the crystalline electrons in bands *i*, *j*,…,with energies $E_i, E_j, \ldots$,etc. The $\vec{k}$ integration is over the entire first Brillouin zone, and *H* is the Hamiltonian interaction.

3. The theorem regarding the semi-classical heat equation

Let's try and prove the following theorem: suppose we have a solid sample (parallelepiped) consisting of layered media, $k_i(x)=k(x_i)+m_i(x-x_i)$, where $, x\in[x_i, x_{i+1}]$ with $, i=0,1,2,\ldots,n-1,$ and that the sample is heated by a multi-mode laser beam ({*m*,*n*}, where *m* and *n* are the order of the Hermite-Gauss modes. Suppose that the source term: $f(x,y,z,t)=f(x,y,z)\cdot[h(t)-h(t-t_0)]$ and the boundary conditions are at the interfaces (here *h* is the step function, *t* is the time and t_0 is the irradiation time):

$$T_{i-1,j,k,l}(x,y,z,t)\big|_{x=x_i} = T_{i,j,k,l}(x,y,z,t)\big|_{x=x_i}$$
$$T_{i+1,j,k,l}(x,y,z,t)\big|_{x=x_{i+1}} = T_{i,j,k,l}(x,y,z,t)\big|_{x=x_{i+1}},$$
$$k_{i-1}\cdot T_{i-1,j,k,l}{}'(x,y,z,t)\big|_{x=x_i} = k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{x=x_i}, \quad (1)$$
$$k_{i+1}\cdot T_{i+1,j,k,l}{}'(x,y,z,t)\big|_{x=x_{i+1}} = k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{x=x_{i+1}}.$$

At the margins of the sample, we consider:

$$k_0\cdot T_{0,j,k,l}{}'(x,y,z,t)\big|_{x=x_0} = h_0\cdot T_{0,j,k,l}(x,y,z,t)\big|_{x=x_0},$$
$$k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{y=y_2/2} = -h_i\cdot T_{i,j,k,l}(x,y,z,t)\big|_{y=y_2/2},$$
$$k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{y=-y_2/2} = h_i\cdot T_{i,j,k,l}(x,y,z,t)\big|_{y=-y_2/2}, \quad (2)$$
$$k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{z=z_3/2} = -h_i\cdot T_{i,j,k,l}(x,y,z,t)\big|_{z=z_3/2},$$
$$k_i\cdot T_{i,j,k,l}{}'(x,y,z,t)\big|_{z=-z_3/2} = h_i\cdot T_{i,j,k,l}(x,y,z,t)\big|_{z=-z_3/2},$$
$$k_n\cdot T_{n,j,k,l}{}'(x,y,z,t)\big|_{x=x_n} = -h_n\cdot T_{n,j,k,l}(x,y,z,t)\big|_{x=x_n},$$

where h_0, h_i and h_n are the surface heat transfer coefficients (for a detailed discussion about *h*, see reference 15, Appendix B). Under these circumstances the theorem says that the heat equation:

$$\nabla\big(k(x,y,z)\nabla T(x,y,z,t)\big)-\rho c\frac{\partial T(x,y,z,t)}{\partial t} = -f(x,y,z,t),$$

which for *k(x,y,z)=k(x)* becomes:

$$\frac{1}{k(x)}\frac{\partial}{\partial x}\left(k(x)\frac{\partial T}{\partial x}\right)+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}-\frac{1}{\gamma}\frac{\partial T}{\partial t} = -\frac{f(x,y,z,t)}{k(x)}, \quad (3)$$

where *k* - the thermal conductivity of the sample; γ - the thermal diffusivity of the sample. It has a rigorous semi-analytical solution, of the form:

$$T_i(x,y,z,t)=\sum_{n_{ph}}\Big(\sum_{m,n}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{1}{(\lambda_j^2+\varepsilon_l^2+\mu_k^2)}[1-e^{-\gamma\cdot(\lambda_j^2+\varepsilon_l^2+\mu_k^2)t}-(1-e^{-\gamma\cdot(\lambda_j^2+\varepsilon_l^2+\mu_k^2)(t-t_0)})h(t-t_0)]\times$$
$$g(\lambda_j,\mu_k,\varepsilon_l)\times\overline{K}_{ij}(\lambda_j,x)\times\overline{K}_k(\mu_k,y)\times\overline{K}_l(\varepsilon_l,z)\Big)\equiv\sum_{n_{ph}}T_{i,n_{ph}}(x,y,z,t) \quad (4)$$

where $\lambda_j, \mu_k, \varepsilon_l$ are the eigenvalues of the eigenfunctions:

$$\overline{K}_l(\varepsilon_l, z)=\cos(\varepsilon_l\cdot z)+\frac{h_i}{k_i\varepsilon_l}\sin(\varepsilon_l\cdot z) \quad ;$$
$$\overline{K}_k(\mu_k, y)=\cos(\mu_k\cdot y)+\frac{h_i}{k_i\mu_k}\sin(\mu_k\cdot y) \quad ;$$
$$\overline{K}_{ij}(x,\lambda_i)=A_iJ_0\left(\frac{2\lambda_j\sqrt{\mu_i(k(x_i)+m_ix)}}{|m_i|}\right)+B_iY_0\left(\frac{2\lambda_j\sqrt{\mu_i(k(x_i)+m_ix)}}{|m_i|}\right), j\in N$$

with : $\mu_i=\rho_i c_i$. (5)

Here: ρ_i is the mass density; c_i is the heat capacity; J_0, Y_0 are the Bessel respectively the Weber functions. We have:

$$g(\lambda_j,\mu_k,\varepsilon_l)=\frac{1}{C(\lambda_j)C(\mu_k)C(\varepsilon_l)}\times$$
$$\sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}}\int_{-y_2/2}^{y_2/2}\int_{-z_3/2}^{z_3/2}f_i(x,y,z,t)\cdot\overline{K}_{ij}(\lambda_j,x)\cdot\overline{K}_k(\mu_k,y)\cdot\overline{K}_l(\varepsilon_l,z)dxdydz \quad (6)$$

Assume that: $y\in[-y_2/2, y_2/2]$ and $z\in[-z_3/2, z_3/2]$. For the constants, we have: $C(\lambda_j)=\sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}}\overline{K}_{ij}^2(x_i,\lambda_j)dx$ and analogue formulas for the others two constants [34].

The indexes *m* and *n*, in equation (4), take into account the decoupled Hermite-Gauss spatial modes. The function $f_i(x,y,z,t)$, in equation (6), is the heat rate produced by the laser beam in solid, and is given by the following formula: $f_i(x,y,z,t)=\alpha_{n_{ph},i}I_{mn}^{n_{ph},i}[h(t)-h(t-t_0)]$, where, as we showed in the previous chapter, $\alpha_{n_{ph},i}$ is the n_{ph}-photon absorption coefficient and $I_{mn}^{n_{ph},i}$ is the Hermite-Gauss intensity of order (m,n) in the layer *i*. Formula (4) defines the temperature $T_{i,n_{ph}}(x,y,z,t)$, which is the temperature field determined only by the absorption of n_{ph}-photon in the layer *i*. Demonstration of the theorem is given in chapter 4.

4. The demonstration of the theorem

Demonstration of the theorem starts with the observation that the heat equation is linear and therefore it is enough to demonstrate the theorem for one single mode (*m* ,*n*) and for a given number of photons interaction.

For a single layered media the heat equation is

$$\frac{\partial}{\partial x}\left(\frac{K_i(x)}{\rho_i c_i}\frac{\partial T_i}{\partial x}\right)+\frac{K_i(x)\partial^2 T}{\partial y^2}+ + \frac{K_i(x)\partial^2 T}{\partial z^2}-\frac{\partial T_i}{\partial t}=-\frac{f_i(x,y,z,t)}{\rho_i c_i} \tag{7}$$

where: $x\in[x_i,x_{i+1}]$.

Apply the integral transform $\overline{K}_{ij}(\lambda_j,x_i)$ which satisfies the equation:

$$\frac{\partial}{\partial x}\left(\frac{K_i(x)}{\rho_i c_i}\frac{\partial\overline{K}_{ij}(\lambda_j,x)}{\partial x}\right)+\lambda_j^2\overline{K}_{ij}(\lambda_j,x)=0 \tag{8}$$

One can check by direct algebraic calculation, that:

$$\overline{K}_{ij}(x,\lambda_i)=A_iJ_0\left(\frac{2\lambda_j\sqrt{\mu_i(k(x_i)+m_ix)}}{|m_i|}\right)+B_iY_0\left(\frac{2\lambda_j\sqrt{\mu_i(k(x_i)+m_ix)}}{|m_i|}\right),j\in N \tag{9}$$

Applying the operator $\overline{K}_{ij}(\lambda_j,x)$ to equation (7), obtain

$$\lambda_j^2\overline{T}_i(\lambda_j,y,z,t)+\frac{\partial^2\overline{T}_i}{\partial y^2}+\frac{\partial^2\overline{T}_i}{\partial z^2}+\frac{\partial\overline{T}_i}{\partial t}=\frac{\bar{f}_i(\lambda_j,y,z,t)}{\rho_i c_i} \quad \text{where:} \tag{10}$$

and

$$\overline{T}_i(\lambda_j,y,z,t)=\frac{1}{C(\lambda_j)}\int_{x_i}^{x_{i+1}}T_i(x,y,z,t)\overline{K}_{ij}(\lambda_j,x)dx \tag{11}$$

$$\bar{f}_i(\lambda_j,y,z,t)=\frac{1}{C(\lambda_j)}\int_{x_i}^{x_{i+1}}f_i(x,y,z,t)\overline{K}_{ij}(\lambda_j,x)dx .$$

Here [34]: $C(\lambda_j)=\sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}}\overline{K}_{ij}^2(x_i,\lambda_j)dx\cdot$ (13)

In the same way, one can apply the functions: $K_k(\mu_k,y)$ and $K_l(\varepsilon_l,z)$, which satisfy the equations:

$$\begin{aligned}&\frac{\partial^2\overline{K_y}(\mu_k,y)}{\partial y^2}+\mu_k^2\overline{K_y}(\mu_k,y)=0\\&\frac{\partial^2\overline{K_z}(\varepsilon_l,z)}{\partial z^2}+\varepsilon_l^2\overline{K_z}(\varepsilon_l,z)=0\end{aligned} \tag{14}$$

Is obtained the following equation:

$$\lambda_j^2\hat{T}_i(\lambda_j,\mu_k,\varepsilon_l,t)+\mu_k^2\hat{T}_i(\lambda_j,\mu_k,\varepsilon_l,t)+ +\varepsilon_l^2\hat{T}_i(\lambda_j,\mu_k,\varepsilon_l,t)+\frac{\partial\hat{T}_i(\lambda_j,\mu_k,\varepsilon_l,t)}{\partial t}=\frac{\hat{f}_i(x,y,z,t)}{\rho_i c_i} \tag{15}$$

were for example:

$$\hat{T}_i(\lambda_j,\mu_k,\varepsilon_l,t)=\frac{1}{C(\lambda_j)C(\mu_k)C(\varepsilon_l)}\times \times\int_{x_i}^{x_{i+1}}\int_{-y_2/2}^{y_2/2}\int_{-z_3/2}^{z_3/2}T(x,y,z,t)\cdot\overline{K}_{ij}(\lambda_j,x)\cdot\overline{K}_k(\mu_k,y)\cdot\overline{K}_l(\varepsilon_l,z)dxdydz \tag{16}$$

In order to eliminate the time parameter apply the direct and inverse Laplace transform to the (15) equation. If we have, like in most cases: $f(x,y,z,t)=f(x,y,z)\cdot[h(t)-h(t-t_0)]$, than one can obtain the solution given in the present article.

5. Conclusions

As a conclusion we can say that the semi-classical heat equation which considers the multi-photon absorption for the laser-solid interaction was solved. The solid is supposed to be layered , each layer having a linear thermal conductivity ($k_i(x)=k(x_i)+m_i(x-x_i)$, where , $x\in[x_i,x_{i+1}]$ with , $i=0,1,2,...,n-1$) . One can choose $m_i=0$, $i=0,1,2,...,n-1$ and obtain a layered structure with constant thermal conductivity on each layer. Another possibility is to take $m_i\neq 0$ for a given *I* and thus to obtain a thermal conductivity which can describe, very close to reality, an interface between two layers.

From a practical point of view, the eigenvalues can be obtained from the boundary conditions [34]. Also the constants A_i, B_i can be obtained easily from the same boundary conditions. One may ask if the proposed model could have practical applications. The answer is positive.

Nonlinear spectroscopy has proved to be invaluable in determining the optical and electronic properties of crystalline solids; e.g., when one-photon absorption is forbidden by selection rules, a higher-order multi-photon absorption may be allowed. Even when one-photon absorption is allowed, because most of the experimentally studied properties are characteristic to the surface rather than to the volume as a consequence of the drastic attenuation of radiation as it propagates into the sample. Multi-photon experiments, on the other hand, can enable the study on the properties of the crystalline volume, because of the significantly smaller values of the multi-photon coefficients. In a recent paper [35], we have calculated the thermal field produced by two-photon absorption coefficient. The conclusion was that the thermal field is detectable by experiments, even when one-photon absorption is present. So, we solved the semi-classical heat equation for laser-solid interaction, introducing quantum physics effects in the source term.

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