

SIMULATION OF THE THERMAL FIELD DISTRIBUTION IN SOLIDS UNDER SHORT LASER PULSES IRRADIATION

M. Oane, D. Apostol*, Ileana Apostol, D. Sporea, V. Damian

National Institute for Laser, Plasma and Radiation Physics, Laser Dept., P.O. Box Magurele-36, RO 76900, Bucharest, Romania

In this paper we have developed an analytical model to study the temperature distributions in IR optical materials heated by laser pulses. Our model takes into account the two-photon absorption. The calculations are based on a three dimensional model of heat diffusion in solids using the integral transform method. We find out the rigorous analytical expression of the thermal field when one considers both: one and two photon absorption. The model is valid for any laser-solid system whose interaction can be described by generalized Beer-Lambert law. Specific results are presented for an application of the model to InSb sample. We find out that two-photon absorption can produce detectable temperature variation.

(Received January 30, 2003; accepted after revision May 8, 2003)

Keywords: Two-photon absorption, Temperature profile, IR optical material, Computer simulation

1. Introduction

Multiphoton absorption (MPA) processes in semiconductors have been the subject of extensive theoretical and experimental investigations since the advent of the laser over four decades ago. Nonlinear absorption plays a crucial role in the high-power laser technology, as well as in many fundamental aspects of solid-state physics.

Moreover, in the last decade the employment of semiconductor components as nonlinear elements in optical communication and information processing systems become very extensive, a more precise and accurate knowledge of their nonlinear optical properties is needed. This is why we consider in this context, the study of two-photon absorption (TPA) coefficients in crystalline solids can be of an unambiguous practical importance for a wealth of applications.

For example, TPA proved to be a powerful spectroscopic tool; first, it is the only method available in the cases when one-photon absorption is forbidden by the selection rules, and second, it gives complementary material information even in the cases in which the linear absorption is allowed, because it permits the study of the crystalline volume and not only of its surface. TPA processes can also give fundamental information about the energy-band structures not easily obtained by using linear techniques.

During the last ten years advances in laser processing have encouraged the development of model calculations of spatial and temporal temperature fields in laser heated solids. In recent years the integral transform method has been successfully applied to the studies of thermal fields in laser-solid interaction [1-4]. Elaborated mathematical models, both analytical and numerical, have been developed to describe the heat flow under a large number of simplifying approximations and assumptions regarding the laser beam and the sample.

The rapid development of the high-power cw and pulsed CO₂ lasers is limited more and more by the susceptibility of windows and mirrors to damage. Ideal high-power laser window material

* Corresponding author: apostold@ifin.nipne.ro

would have low absorption coefficient at the laser wavelength. In this paper we consider the heating of a solid sample by laser pulses. In order to understand better the physical absorption process it is necessary to consider multi-photon processes. We will take into account one and two-photon absorption coefficients. Three-photon absorption has been relatively less well studied than two-photon absorption because of the significantly smaller transition probability associated with it. From theory and experiment we know that the higher-order multiphoton transition probabilities decrease rapidly with increasing order.

The role of two-photon absorption in semiconductors is of increasing importance as semiconductors components become employed as nonlinear elements in optical communications and information processing systems. Two-photon absorption provides a fundamental limitation for all optical switching in the transparent spectral region of semiconductors. Two-photon absorption has also potential applications as a nonlinear spectroscopic technique, providing complementary material information to one-photon-absorption measurements.

We carry out three-dimensional model calculations in which full account is taken not only of the two-photon absorption but also of the time and space characteristic of the laser beam as the heating source. We discuss the influence of the two-photon absorption coefficient in establishing the thermal profiles. We also discuss the influence of the heat transfer coefficient.

2. The analytical model

In the present paper, the macroscopic heat equation, is employed to investigate the temperature field in a semiconductor [5-7] exposed to a Gaussian or flat spatial profile and a rectangular nanosecond pulse. The sample is supposed to be homogeneous and therefore there is no angular dependence of the temperature variation. The equation describing the heat diffusion inside a cylindrical IR optical material irradiated by a laser beam centered to the probe is fully described by the partial differential equation:

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

where k - the thermal conductivity of the sample; γ - the thermal diffusivity of the sample ($\gamma = \frac{k}{c \cdot \rho}$); c - the heat capacity of the sample; ρ - the mass density of the sample. Here $A(r, z, t)$ represents the heat rate (per unit volume and time) produced by the laser in the sample. The temperature T is a function of (r, z, t) and is defined here as a temperature variation rather than an absolute temperature: $T(r, z, t) = T_{fi} - T_{in}$, where T_{fi} and T_{in} are the final and the initial absolute temperature of the sample. If we consider a linear heat transfer at the sample surface (the "radiation" boundary condition), we have:

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

where h - heat transfer coefficient of the sample surface a, b - thickness and respectively the radius of the sample. In the presence of both one- and two-photon absorption, described by coefficients α and β respectively, the change in the intensity of the light as it passes through the sample is given by generalized Beer-Lambert law [8]: $\frac{dI}{dz} = -\alpha \cdot I - \beta \cdot I^2$ when free carrier absorption is negligible. Two-photon absorption coefficient can be calculated in second-order perturbation theory

in terms of transition probabilities W_2 : $\beta = 4W_2\hbar\omega/I^2$. The transition probability from an initial valence band to a final conduction band, accompanied by the simultaneous absorption of two photons, each of frequency ω can be calculate as:

$$W_2 = \frac{2\pi}{\hbar} \int \left| \frac{\sum_i \langle \psi_c | H | \psi_i \rangle \langle \psi_i | H | \psi_v \rangle}{(E_i - E_v - \hbar\omega)} \right|^2 \times \delta(E_c(\vec{k}) - E_v(\vec{k}) - 2\hbar\omega) \frac{d^3\vec{k}}{(2\pi)^3} \quad (3)$$

In above equation ψ_i is the Bloch function of the crystalline electrons in band i whose energy is E_i and H is the interaction Hamiltonian. The calculation of numerical values for two-photon transition probability is extremely difficult. The straightforward solution to the Beer-Lambert equation is [8, 9]:

$$\frac{I}{I_0} = \frac{(1-R)^2 \exp(-\alpha z)}{1 + \beta \cdot I_0 (1-R) [1 - \exp(-\alpha z)] / \alpha}, \quad (4)$$

where R is the reflectivity at the wavelength of the incident radiation and z is the thickness of the sample.

In order to take into account the two photon absorption, the heat rate per unit volume and time will be determined by the laser intensity, according to Beer-Lambert's law:

$$A(r, z, t) = (\alpha \cdot I_{00}(r, z) + \beta I_{00}^2(r, z)) \cdot (h(t) - h(t - t_0)), \quad (5)$$

where t_0 is the pulse duration and $h(t)$ is the step function.

The solution of the heat equation is (Appendix A):

$$T_{\alpha\beta}(r, z, t) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \left[\frac{1}{\mu_i^2 + \lambda_j^2} \cdot f_{\alpha,\beta}(\mu_i, \lambda_j) \cdot (1 - e^{-\theta_{ij}^2 t} - (1 - e^{-\theta_{ij}^2(t-t_0)}) \cdot h(t-t_0)) \right] \\ \times K_r(\mu_i, r) \cdot K_z(\lambda_j, z) \quad (6)$$

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

$$f_{\alpha,\beta}(\mu_i, \lambda_j) = \frac{1}{kC_i C_j} \int_0^a \int_0^b (\alpha I_{00} + \beta I_{00}^2) r \cdot K_r(\mu_i, r) \cdot K_z(\lambda_j, z) dr dz \quad (7)$$

The coefficients C_i and C_j are normalizing coefficients. The eigenvalues μ_i and λ_j correspond to the eigenfunctions $K_r(r, \mu_i)$ and $K_z(z, \lambda_j)$. The integral operators corresponding to the eigenfunctions $K_r(r, \mu_i) = J_0(\mu_i \cdot r)$ and $K_z(z, \lambda_j) = \cos(\lambda_j z) + \frac{\hbar}{\lambda_j \cdot k} \sin(\lambda_j \cdot z)$ are normalized by the following coefficients:

$$C_i = \int_0^b r K_r^2(r, \mu_i) dr = \frac{b^2}{2\mu_i^2} \left(\frac{\hbar^2}{k^2} + \mu_i^2 \right) J_0^2(\mu_i b) \quad \text{and} \\ C_j = \int_0^a K_z^2(z, \lambda_j) dz = \frac{1}{4\lambda_j^3} \left(2\frac{\hbar}{k} \lambda_j + 2a \frac{\hbar^2}{k^2} \lambda_j + 2a \lambda_j^3 - 2\frac{\hbar}{k} \lambda_j \cos[2a\lambda_j] \right. \\ \left. - \frac{\hbar^2}{k^2} \sin[2a\lambda_j] + \lambda_j^2 \sin[2a\lambda_j] \right) \quad (8)$$

The eigenvalues μ_i and λ_j are determined from the boundary conditions by the following equations [1]:

$$\begin{aligned} \frac{h}{k} J_0(\mu_i b) - \mu_i J_1(\mu_i b) &= 0 \text{ and} \\ 2 \cdot \cot(\lambda_j a) &= \frac{\lambda_j \cdot k}{h} - \frac{h}{\lambda_j k} \end{aligned} \quad (10)$$

3. Results and discussion

In the previous section the heat diffusion equation was analytically solved in order to determine the temperature field inside a semiconductor sample. One cylindrical sample made of InSb was considered and its dimensions are the radius $b=10$ mm and the thickness $a=4$ mm. The sample was supposed to be irradiated by a 250 ns TEM₀₀ CO₂ laser beam with the power 100 W and 2 mm width.

The InSb sample has the following characteristics: mass density: $\rho = 5.78$ g/cc; thermal conductivity $k = 16$ W/m K; specific heat $c = 0.144$ J/g °C; absorption coefficient $\alpha = 0.64$ mm⁻¹; two-photon absorption coefficient $\beta = 15$ cmMW⁻¹[5,6,7,9]. The temperature fields plotted in Figs. 1-4, correspond to $z = 0$, $h = 6 \times 10^{-7}$ Wmm⁻²K and a null surface absorption.

A typical temperature distribution versus time and radial coordinate for 250 ns TEM₀₀ CO₂ laser beam is shown in Fig. 1. The temperature distribution reaches its maximum in the sample center, at the point where the power density has its maximum.

The same temperature field is presented in Fig. 2, but for a 0.2 ms TEM₀₀ CO₂ laser beam with 50 W power. As we expected the general shape of the thermal fields are very similar but the pulse duration of the laser beam determines the temporal evolution of the temperature field. One can easily notice that in Fig. 1 the cooling process is faster in comparison with the one in Fig. 2.

In Fig. 3 is presented the same temperature field as in Fig. 1 but for $h = 3 \times 10^{-7}$ Wmm⁻²K. One can easily observe the general increase in temperature but the shape of the field temperature remains the same. The explanation is that h is the key factor which determines the energy losses by radiation and convection through the surface, and therefore

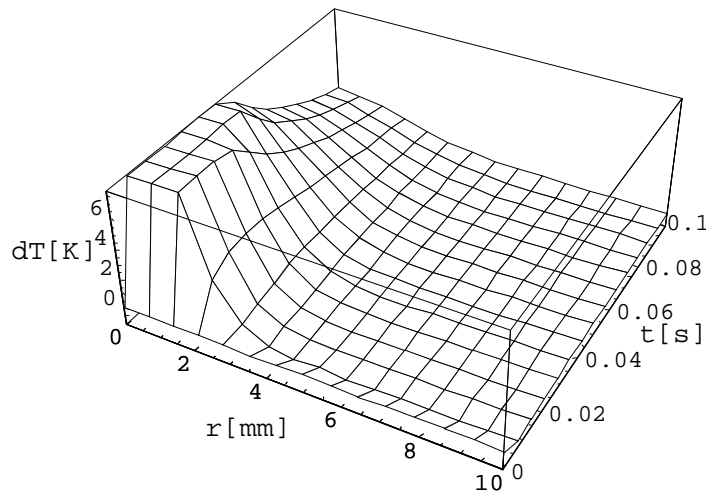


Fig. 1. Computed temperature field inside InSb probe exposed 250 ns to a 100 W TEM₀₀ CO₂ laser beam.

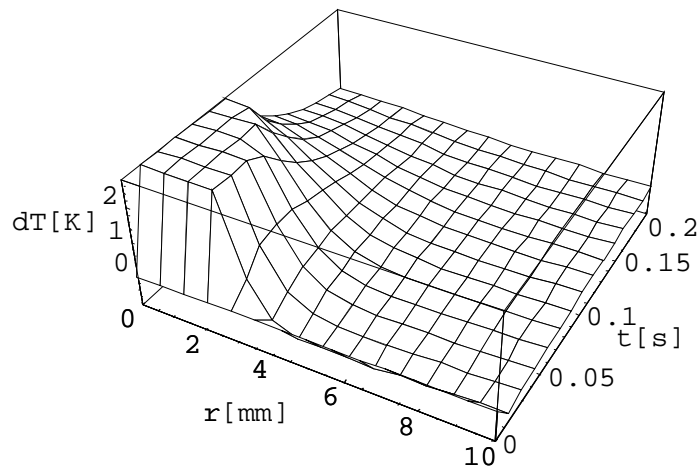


Fig. 2. Computed temperature field inside InSb probe exposed for 0.2 ms to a 50 W TEM₀₀ CO₂ laser beam.

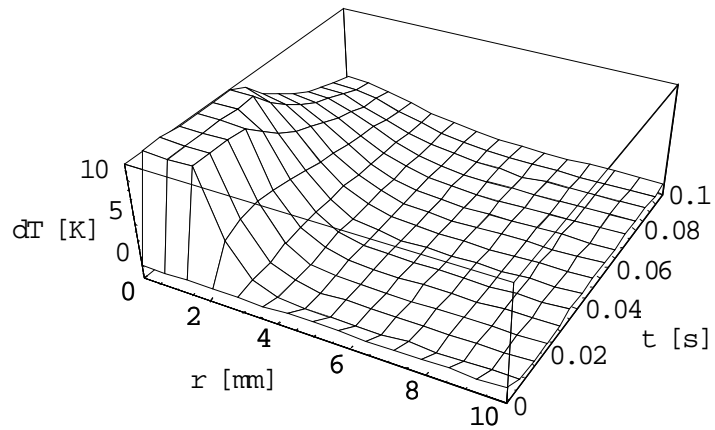


Fig. 3. Computed temperature field inside InSb probe with $h = 3 \times 10^{-7} \text{ Wmm}^{-2}\text{K}$, exposed for 250 ns to a 100 W TEM₀₀ CO₂ laser beam.

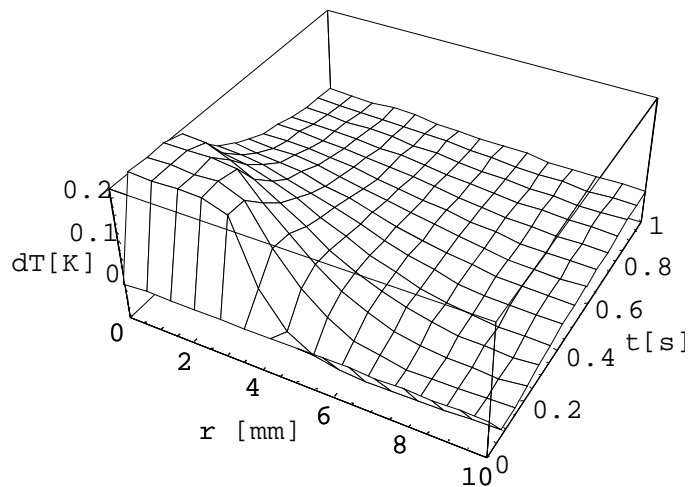


Fig. 4. Computed temperature field inside InSb probe exposed for 250 ns to a 100 W TEM₀₀ CO₂ laser beam, when $\alpha = 0$ and the two-photon absorption coefficient $\beta = 15 \text{ cmMW}^{-1}$.

establish the steady state regime where there is an equilibrium between the energy absorbed from the laser and the energy losses.

We present in Fig. 4 the temperature field produced only by the two-photon absorption coefficient ($\alpha=0$). One can notice that the temperature field is less than five percent from the maximum temperature field produced in the case $\alpha \neq 0$ (Fig. 1).

4. Summary

The model applied in this paper is one which assumes that the laser beam interacts with the sample via one- and two-photon absorption coefficient. Our study concludes that for solid materials, the heat equation has a rigorous analytical expression, and the two-photon absorption produce a detectable temperature field in comparison with the field produced by the one-photon absorption.

The temperature profile model could be applied to any other semiconductor introducing the specific constants of the material.

Appendix A

The heat equation inside the sample (Eq. (1)) is solved using the integral operators method. To eliminate differentiation with respect to r , we set: $D_r = \partial^2 / \partial r^2 + (1/r)(\partial / \partial r)$.

The auxiliary function $K_r(\mu_i, r)$ must satisfy the equation:

$$\frac{\partial^2 K_r}{\partial r^2} + \frac{1}{r} \frac{\partial K_r}{\partial r} + \mu^2 K_r = 0 \quad (\text{A.1})$$

and from the first equation representing the boundary conditions

$$(\text{Eq. (2)}): k \frac{\partial K_r(r, z, t)}{\partial r} \Big|_{r=b} + h K_r(b, z, t) = 0 \quad (\text{A.2})$$

The solutions of Eq. (A.1) are $K_r(r, \mu_i) = J_0(\mu_i r)$ where $J_n(x)$ is the Bessel function.

We have: $\tilde{K}_r(r, \mu_i) = J_0(\mu_i r) \cdot r \cdot (1/C_i)$ Here: $C_i = \int_0^b r K_r^2(r, \mu_i) dr = \frac{b^2}{2\mu_i^2} \left(\frac{h^2}{k^2} + \mu_i^2 \right) J_0^2(\mu_i b)$.

The eigenvalues μ_i corresponding to the eigenfunctions K_r are calculated by solving the next equation that comes from the border conditions (Eq. A.2): $\frac{h}{k} J_0(\mu_i b) - \mu_i J_1(\mu_i b) = 0$.

Applying $\tilde{K}_r(r, \mu_i)$ Eq. (1) becomes:

$$-\mu_i^2 \tilde{T} + \frac{\partial^2 \tilde{T}}{\partial z^2} - \frac{1}{\gamma} \frac{\partial \tilde{T}}{\partial t} = -\frac{\tilde{A}(\mu_i, z, t)}{k} \quad (\text{A.3})$$

Here: $\tilde{T}(\mu_i, z, t) = \frac{1}{C_i} \int_0^b T(r, z, t) \cdot r \cdot J_0(\mu_i r) dr$ and $\tilde{A}(\mu_i, z, t) = \frac{1}{C_i} \int_0^b A(r, z, t) \cdot r \cdot J_0(\mu_i r) dr$

To eliminate differentiation with respect to z , we set: $D_z \tilde{T} = \frac{\partial^2 \tilde{T}}{\partial z^2}$.

The auxiliary function $K_z(\lambda_j, z)$ must satisfy the equation:

$$\frac{\partial^2 K_z}{\partial z^2} + \lambda^2 K_z = 0 \quad (\text{A.4})$$

and the boundary conditions (from Eq(2)) : $[k(\frac{\partial K_z}{\partial z}) - hK_z]_{z=0} = 0$ and $[k(\frac{\partial K_z}{\partial z}) + hK_z]_{z=a} = 0$

We have : $K_z(z, \lambda_j) = \cos(\lambda_j z) + \frac{h}{\lambda_j k} \sin(\lambda_j \cdot z)$ and $\tilde{K}_z(z, \lambda_j) = \frac{1}{C_j} K_z(z, \lambda_j)$

Here: $C_j = \int_0^a K_z^2(z, \lambda_j) dz$. From the boundary conditions we obtained: $2 \cdot \cot(\lambda_j a) = \frac{\lambda_j k}{h} - \frac{h}{\lambda_j k}$.

Applying $\tilde{K}_z(z, \lambda_j) = \frac{1}{C_j} K_z(z, \lambda_j)$ Eq. (A.3) becomes:

$$(\mu_i^2 + \lambda_j^2) \bar{T} + \frac{1}{\gamma} \frac{\partial \bar{T}}{\partial t} = \frac{\bar{A}(\mu_i, \lambda_j, t)}{k} \quad (\text{A.5})$$

where: $\bar{T}(\mu_i, \lambda_j, t) = \frac{1}{C_i C_j} \int_0^a \int_0^b T(r, z, t) \cdot r \cdot K_r(\mu_i, r) \cdot K_z(\lambda_j, z) dr dz$ and

$$\bar{A}(\mu_i, \lambda_j, t) = \frac{1}{C_i C_j} \int_0^a \int_0^b A(r, z, t) \cdot r \cdot K_r(\mu_i, r) \cdot K_z(\lambda_j, z) dr dz \quad (\text{A.6})$$

Taking into account Eq. (5) and using the direct and inversion Laplace transform technique one can solve (A.6) and the solution (6) given in this article will be obtained.

References

- [1] T. Visan, D. Sporea, G. Dumitru, *Infrared Physics & Technology* **39**, 335 (1998).
- [2] M. Oane, D. Sporea, *Infrared Physics & Technology* **42**, 31 (2001).
- [3] M. Oane, D. Sporea, *SPIE Proc. Vol. 4430*, 898 (2001).
- [4] N. S. Koshlyakov, M. N. Smirnov, E. B. Gliner, *Differential Equations of Mathematical Physics*, North-Holland Publishing, Amsterdam, 1964.
- [5] J. M. Doviak, A. F. Gibson, M. F. Kimmitt, A. C. Walker, *J. Phys. C: Solid State Phys.* **6**, 593 (1973).
- [6] C. C. Lee, H. Y. Fan, *Appl. Phys. Lett.* **20**(1), 18 (1972).
- [7] A. Miller, A. Johnston, J. Dempsey, J. Smith, C. R. Pidgeon, G. D. Holan, *J. Phys. C: Solid State Phys.* **12**, 4839 (1979).
- [8] M. Dabbicco, I. M. Catalano, *Optics Communications* **178**, 117 (2000).
- [9] A. Vaidyanathan, A. H. Guenther, S. S. Mitra, *J. Opt. Soc. Am. B/Vol. 2*(2), 300 (1985).