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The applicability of the Fourier heat equation for study of nano particles clusters

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The solution of the presented problem for detecting and describe nano-particles-clusters, which are inside of a metal. The solution is based on the heat equation which solved using the integral transform technique in order to improve the more inexact results obtained by the first Born approximation, Green function method, or pure numerical methods. In this work we present the solutions for 1, 2 and 4 nano-particles-clusters in 3D graphical form.

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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] applications. In all these areas of applications, the laser-solid interaction played a crucial role. The theory of heat conduction was naturally applied to explain this interaction since it was well studied for a long time [2]. For describing this interaction, the classical heat equation was used in a lot of applications. Apart of some criticism [3], the heat equation still remains one of the most powerful tools in describing most thermal effects in laser-solid interactions [4]. In particular, the heat equation can be used for describing both of light interaction with homogeneous [5, 6] and inhomogeneous solids. In the literature, thus a special attention was given to cases of light interaction with multi-layered samples [7] and thin films [8].

2. The statement of the problem

We assume in the following treatment that we have a solid consisting of a layer of a metal such as Au, Ag, Al or Cu, respectively. Assuming that only a photothermal interaction takes place, and that all the absorbed energy is transformed into heat, the linear heat flow in the solid is fully described by the heat partial differential equation:

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

where: T(x,y,z,t) is the spatio-temporal temperature function, γ is the thermal diffusivity, k is the thermal conductivity and A is the volume heat source (per unit time). In general one can consider the linear heat transfer approximation and using the integral transform method assume the following form for the solution of the above heat equation [5,6]:

$$T(x,y,z,t)=\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty} f(\mu_i,\nu_j,\lambda_k)\cdot g(\mu_i,\nu_j,\lambda_k,t) \times K_x(\mu_i,x)\cdot K_y(\nu_j,y)\cdot K_z(\lambda_k,z) \quad (2)$$

where:

$$f(\mu_i,\nu_j,\lambda_k)=\frac{1}{k\cdot C_i\cdot C_j\cdot C_k}\int_0^a\int_{-b}^{b}\int_{-c}^{c} A(x,y,z,t)K_x(\mu_i,x)\cdot K_y(\nu_j,y)\cdot K_z(\lambda_k,z)dxdydz$$

and

$$g(\mu_i,\nu_j,\lambda_k,t)=1/(\mu_i^2+\nu_j^2+\lambda_k^2)[1-e^{-\beta_{ijk}^2 t}-(1-e^{-\beta_{ijk}^2(t-t_0)})\cdot h(t-t_0)] \quad (3)$$

with $\beta_{ijk}^2=\gamma(\mu_i^2+\nu_j^2+\lambda_k^2)$.

Here t_0 is the light pulse length (assumed rectangular) and h is the step function. The functions $K_x(\mu_i,x), K_y(\nu_j,y)$ and $K_z(\lambda_k,z)$ are the eigenfunctions of the integral operators of the heat equation and μ_i,ν_j,λ_k are the eigenvalues corresponding to the same operators. Here for example:

$K_x(\mu_i, x) = \cos(\mu_i \cdot x) + (h_{lin} / k \cdot \mu_i) \cdot \sin(\mu_i \cdot x)$,

with h_{lin} - the linear heat transfer coefficient of the solid sample along x direction.

The coefficients C_i, C_j *and* C_k are the normalizing coefficients where, for example:

$$C_i = \int_{-b}^{b} K_x^2(\mu_i, x) dx \cdot$$

3. The model

We use the thermal parameters of the Cu sample as given in Table 1:

Table 1. Thermal Parameters of Cu.

	K[W/cmK]	γ [cm^2/s]	α [cm^{-1}]
Cu	3.95	1.14	$7.7 \cdot 10^5$

We use the heat equation for a configuration where the layers are assumed to have a thickness of 1mm onto which are included clusters of nano-spheres. The heat term for such a system can be represented by the following equation:

$$A(x,y,z,t) = \sum_{m,n,p} I(x,y,z)((\alpha_1 + r_S\delta(z) + \alpha_{mnp}(\delta(x_m)\cdot\delta(y_n)\cdot\delta(z_p))) \cdot (h(t) - h(t-t_0))$$

where, m,n,p denote the positions of the nano-particles-clusters, α_1 - the optical absorption coefficient, I the incident plane wave radiation intensity incoming from the top –z direction, r_S -the surface absorption coefficient, α_{mnp} -the nano-particles optical absorption coefficients, x,y,t represent the space and time coordinates on the layer surface and h is the step time function.

For our simulation we may consider: $\alpha_{mnp} >> \alpha_1 + r_S d(z)$.

4. Results

Inserting groups or clusters of nano-particles-clusters on top of a layer exposed to irradiation gives a detectable increase of temperature in comparison with the bulk material in pure form. This result can be seen in the following simulations.

For m,n=1,2 and p=1 we have plotted in Fig.1-3, the thermal field of 1,2 and 4 nano-particles-clusters for the case of a Cu layer.

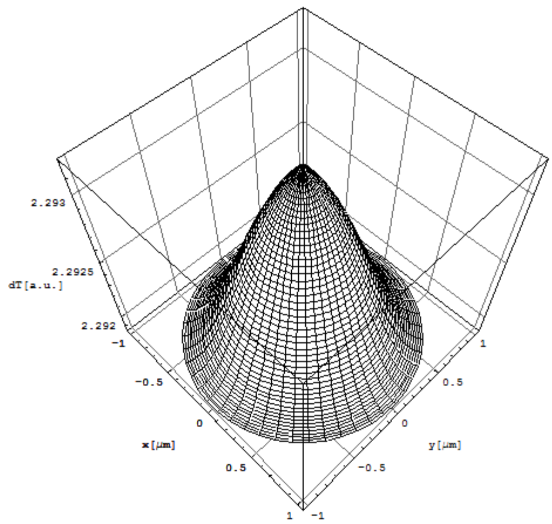

Fig. 1. The thermal field produced by 1 nano-particle-cluster on a Cu substrate. The nano-particle is situated at x=0 and y=0, and 200 nm depth inside Cu sample

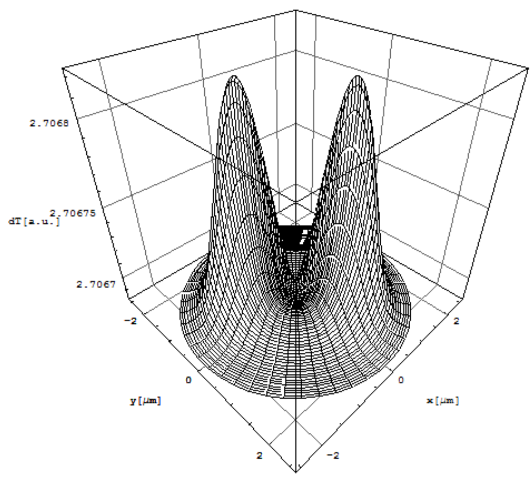

Fig. 2. The thermal field produced by 2 nano-particles-clusters on a Cu substrate. The 2 nano-particles-clusters have the coordinates symmetric in rapport with the heat source. The 2 nano-particles-clustersarealso 200nm inside Cu sample

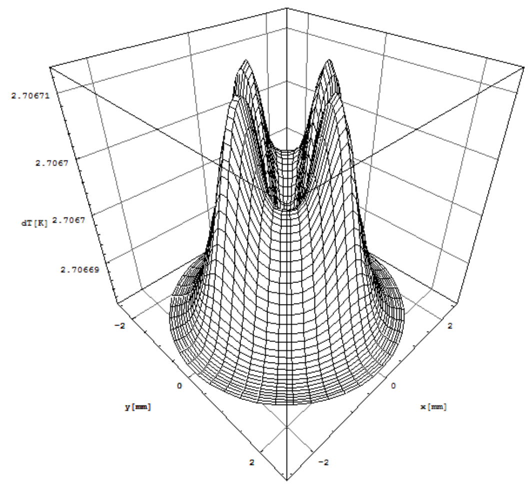

Fig. 3. The thermal field produced by 4 nano-particles-clusters on a Cu substrate. The depth is also 200nm

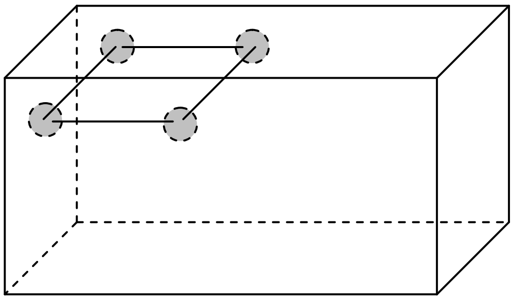

Fig. 4. The "geometrical" situation for the figure number 3

5. Conclusions

The present paper continues the numerous ideas developed in the last years year with the integral transform technique applied to classical Fourierheat equation [8].

From practical point of view consider the formula (2), that*:* ***i***varies from 1 to 100*; j* varies from 1 to 100, and *k* varies from 1 to 100. In consequence we will have the solutions like a sum of 1 million functions. In this way our solutions becomes from semi-analytical into analytical one. The solutions it is easy to compute in MATHEMATICA, or other package software.

In conclusions we consider that the method of integral transform technique is a serious candidate in competition with: Born approximation, Green function method or numerical methods.

The nano-particles-clusters should be of the order of magnitude of 20 nm, which is the limit of availability of Fourier model [9].

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