THE IMPROVEMENT OF THE THERMAL PARAMETERS OF DIFFERENT MATERIALS USING NANO-MATERIALS NETWORKS

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Abstract: *The solution of the presented problem for designing thermo-resistant materials 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. The term of: "thermal black holes" was introduced to represent local sinks for thermal energy. In this work we present the solutions for 1, 2 and 4 nano-particle clusters in 3D graphical form.*

Keywords: *nano-particle clusters, heat equation, integral transform techniques.*

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 has been 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 light interaction with homogeneous [5, 6] and inhomogeneous solids [7]. Thus in literature thus a special attention was given to cases of light interaction with multi-layered samples [8] and thin films [9].

2. The statement of the problem

In the following treatment we assume that we have a solid consisting of a layer of a metal such as Au, Ag, Al or Cu. Assuming that only a photothermal interaction is developing, 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:

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

where: T(*x, y z, t*) is the spatial-temporal temperature function, γ is the thermal diffusivity, *k* is the thermal conductivity and *A* is the volume heat source (per unit time). General one can consider the linear heat transfer approximation and using the integral transform method, may 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: $C_i=\int_{-b}^{b}K_x^2(\mu_i,x)dx$.

3. The model

Thermal parameters of the Cu sample as given in Table 1 were used:

Table 1. Thermal Parameters of Cu.

	K [W/cmK]	γ [cm^2/s]	α [cm^{-1}]
Cu	3.95	1.14	$7.7\cdot10^5$

We used the heat equation for a configuration where the layers are assumed to have a thickness of 10000 nm onto which clusters of nano-spheres each with 100nm radius on top of the surface are included. 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 centroids; 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.

If $\alpha_{mnp} << \alpha_1 + r_S d(z)$ (e.g., about 100 times smaller than the layer optical absorption coefficient), by solving the heat equation one can observe it is possible to obtain "thermal black holes" where the singularities are positioned in each one of the groups of nano-particles.

4. Discussion and conclusions

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

For *m, n*=1, 2 and *p*=1, in Fig.1-3 we have plotted the thermal field of 1, 2 and 4 nano-particles for the case of a Cu layer. Note one "thermal black hole" in Figure 1.

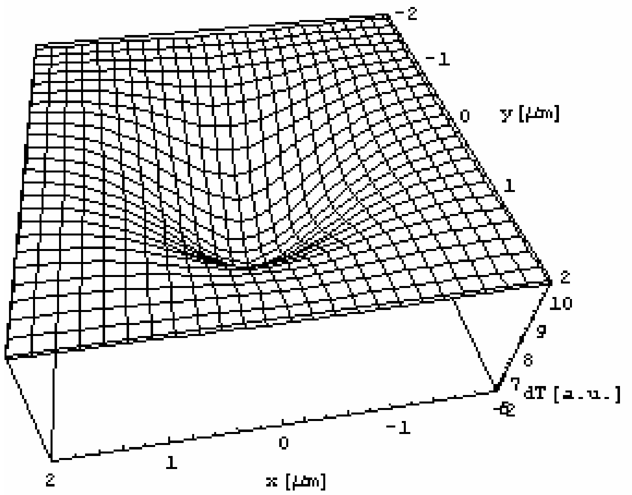

Fig.1. The thermal field produced by 1 nano-particle on a Cu substrate. The nano-particle is situated at x=0 and y=0.

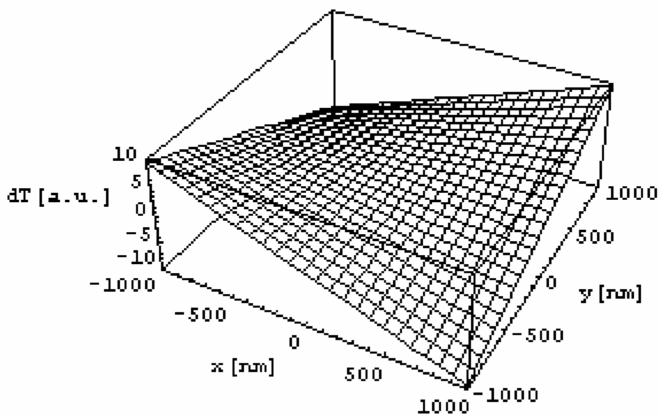

Fig. 2. The thermal field produced by 2 nano-particles on a Cu substrate. The 2 nano-particles have the coordinates: {1000,-1000} and {-1000, 1000}.

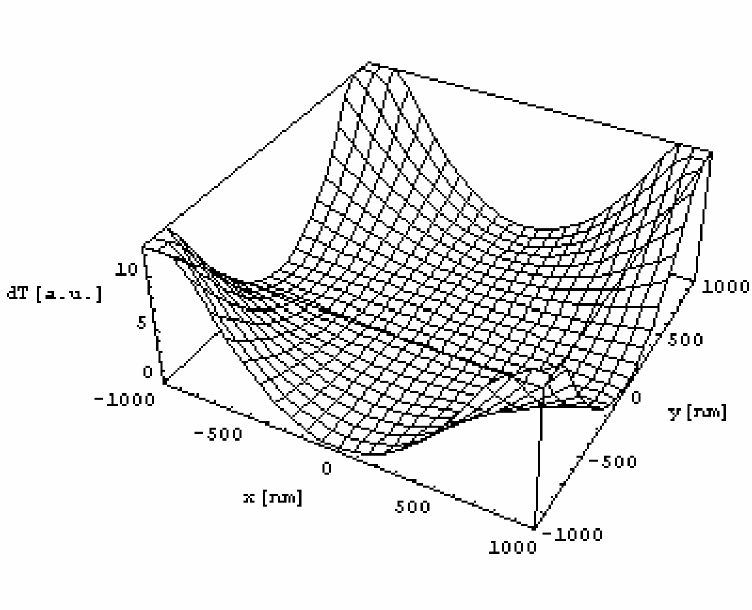

Fig. 3. The thermal field produced by 4 nano-particles on a Cu substrate. The 4 nano-particles have the coordinates: {0,-1000}, {0, 1000}, {-1000,0} and {1000, 0}.

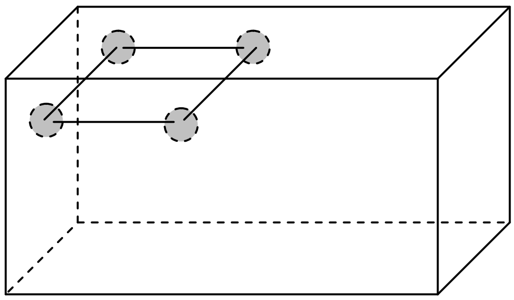

Fig. 4. The "geometrical" positioning for the figure number 3.

As a conclusion, a nano-particle cluster produces quasi-singularities in the heat equation which in a way, is similar with the black-holes in gravitation and one can speculate on the possibility to obtain thermo-resistant materials.

If $\alpha_{mnp} >> \alpha_1 + r_S d(z)$, e.g., about 100 times bigger than the layer optical absorption, we have the situation from figure 5.

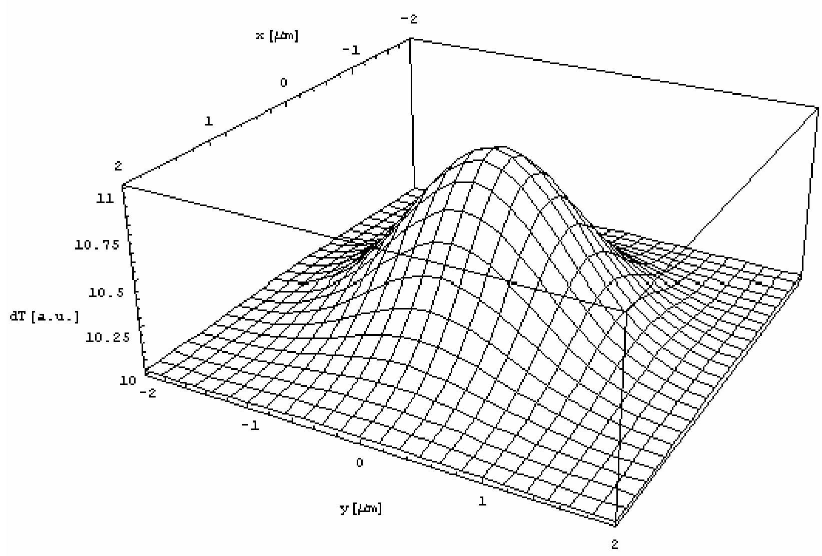

Fig. 5. The thermal field produced by 1 nano-particle on a Cu substrate (the nano-particle is situated at x = 0 and y = 0) when $\alpha_{mnp} >> \alpha_1 + r_S d(z)$.

The nano-particles for figure 1 are, for example, Al_2O_3 or Fe_2O_3 and for figure 5, a good example is Si.

The present paper is continuing the numerous ideas currently developed with the integral transform technique applied to heat equation [10-12].

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