

**ТЕОРИЯ ХИМИЧЕСКОГО СТРОЕНИЯ И РЕАКЦИОННОЙ
СПОСОБНОСТИ ПОВЕРХНОСТИ.
МОДЕЛИРОВАНИЕ ПРОЦЕССОВ НА ПОВЕРХНОСТИ**

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**THERMAL HISTORY DUE TO LASER HEATING
OF SOLID SURFACES**

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Using the finite integral transformation along the spatial Cartesian coordinates, an analytical expression for calculating the temperature distribution $T(x, y, z)$ due to laser pulses in a solid located in the half-space $z < 0$ is obtained. The numerical calculations show that a uniform warming of the body surface takes place only during a part of the pulse duration. Deep inside the solid, the maximum temperature value compared to the surface takes place with a time delay. This time delay depends on the heat wave propagation velocity. Along with heat penetration into the solid, a maximum temperature zone degradation process takes place. Cooling velocity in the upper layers appears to be higher than that in the deeper layers. However, the cooling period in deeper layers is less than that in upper layers. The results obtained are qualitatively consistent with published experimental data.

Introduction

Recently, research for any sort of solid surface structures created by means of laser radiation and/or laser beams interference pattern has essentially been of interest [1-10]. Heating due to laser ablation can be additionally used for the formation of nanosized particles in solid electrolytes [11]. Pulse laser ablation of solid targets in the gas phase has been widely used for the preparation of various nanostructured materials such as nanoparticles, nanotubes and nanocomposites [12-14]. The study of laser-induced heating and melting are of great importance for achieving high quality materials processing when using lasers [15-19]. However, until recently there is a question on the features of the spatial and temporal distribution of temperature due to laser heating of solid surfaces.

In this paper, the distribution of the temperature $T(x, y, z)$ on a solid surface occupying a semi-space of $z < 0$ is studied. A temperature on the surface of the solid is due to streams of energy taken in from the surface due to heat conductivity. The numerical calculations showed that in the deeper layers of the solid the maximum value of the temperature is reached with a delay compared to the surface of the solid. This is due to the heat-wave delay. A rate of cooling of the top layers of the solid appears to be faster than for the deeper layers. In addition, numerical calculations showed that the maximal temperature at a certain depth depends slightly on the form of intensity distribution of the laser beam used.

Statement of the problem

Let us consider the process of heating a solid surface by two-dimensional laser beam interference pattern represented in Fig. 1. It is assumed that the laser beams are identical, fall normally to the surface and the interaction between the beams is negligible. It is also assumed that the thermo-physical characteristics of the medium are independent on the temperature or

spatial coordinates. In this case, the heat diffusion equation describing the distribution of temperature T in the half-space $0 < z < \infty$ can be written as:

$$\frac{\partial T}{\partial t} = \chi \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \frac{\alpha}{\rho c_p} I(x, y, z, t), \quad (1)$$

where t is the time, x, y, z are the Cartesian coordinates, $\chi = \kappa / \rho c_p$ is the thermal diffusivity, κ is the heat conductivity, c_p is the heat capacity, ρ is the density, α is the absorption coefficient, and I is the power density of the laser beam.

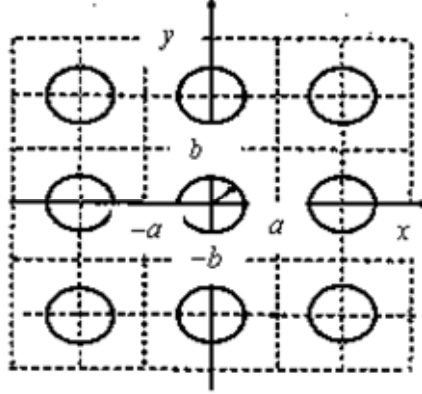


Fig. 1. Two-dimensional periodic structure formed by laser beams.

We assume that a laser beam is represented by the Gaussian intensity distribution:

$$I(x, y, z, t) = H(x, y) I_0 (1 - R) e^{-\alpha z} \exp\left\{-\frac{x^2 + y^2}{r^2}\right\} f(t), \quad (2)$$

where I_0 is the maximum intensity of laser beam, R is the reflection coefficient, r is the radius of one laser beam, $H(x, y) = 1$ if $x^2 + y^2 \leq r^2$, and $H(x, y) = 0$ otherwise, and $f(t)$ is a function which describes the distribution of a laser impulse as time function.

The required distribution of temperatures is subjected to the following initial and boundary conditions:

$$\begin{aligned} T(x, y, z, 0) &= T_0, \\ \frac{\partial T}{\partial x} \Big|_{x=\pm a} &= 0, \quad \frac{\partial T}{\partial y} \Big|_{y=\pm b} = 0, \quad \frac{\partial T}{\partial z} \Big|_{z=0} = 0, \quad \lim_{z \rightarrow \infty} T = T_0, \end{aligned} \quad (3)$$

where $2a, 2b$ are the dimensions of a rectangular pulse period, T_0 is the initial value of the temperature.

The solution of the problem can be constructed using Green functions as it was done by some authors [19, 20]. However, the problem of calculating infinite integrals is not a trivial one, so in the present paper other approach is offered. It may be noticed that the linear equation (1) contains a constant coefficient, and variables that can be divided in the function of the source (2). Under such circumstances, for solving equation (1), infinite integral transformation on coordinates x, y and Fourier transformation on coordinate z can be used. Consecutive performance of these transformations (independent of execution sequence) leads to system of

non-uniform differential equations of the first order over time. The solution of these equations is then straightforward. Using reverse transformation, an analytical solution in the form of converging series and integrals can be then obtained.

Analysis of the general solution and numerical results

Two-dimensional periodic structures are investigated with active sources within the limits of a circle with radius r , and with Gaussian intensity distribution in space. The cases analyzed when the time function $f(t)$ is represented by the Dirac function $\delta(t)$ or Heaviside function $H(t)$. The square cell ($b = a$) is assumed. Dimensionless time is used $t = \chi t' / a^2$ (t' is natural time), also dimensionless temperature $T^* = T / \theta$, where $\theta = \alpha a^2 J_0 / \chi$, and dimensionless space coordinates $x = x' / a$, $y = y' / a$, $z = z' / a$, where x', y', z' are the linear ones.

Some numerical calculation results are shown in Figs. 2 and 3. The data make it possible to get an idea about the temperature distribution in the layers when the time of the laser activity is long enough (stationary solution) depending on the distance z of the layer from the surface of the solid and on the beam radius r . Fig. 2 shows the distribution of a stationary temperature in the location of a heating spot for different beam radii r and some z value.

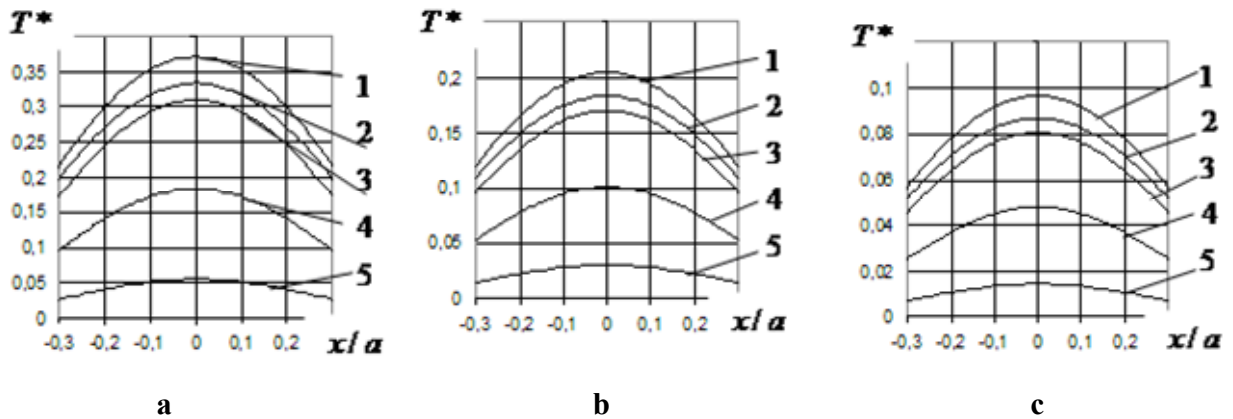


Fig. 2. The temperature (T^*) in the middle section of a solid ($y = 0$) versus the layers distance (z) from its surface and beam radius r for: a – $z = 1$; b – $z = 5$; c – $z = 10$: 1 – $r = 1.0$; 2 – $r = 0.8$; 3 – $r = 0.4$; 4 – $r = 0.4$, 5 – $r = 0.2$.

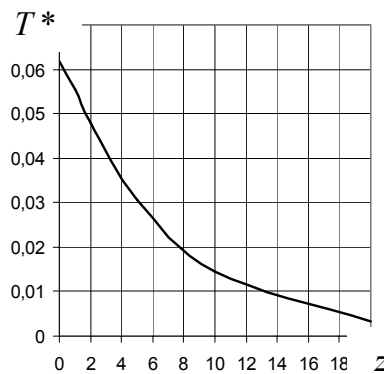


Fig. 3. Stationary temperature T^* versus the distance z from the solid surface.

The calculations were realized using a formula given by:

$$T_{st}(x, y, z) = \frac{2}{\pi ab} I_0(1-R) \frac{\alpha^2}{\chi} \times \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \varepsilon_{nm} \left\{ \left[\frac{\exp(-\alpha z)}{\alpha} - \frac{\exp\left(-\sqrt{\lambda_n^2 + \mu_m^2} z\right)}{\sqrt{\lambda_n^2 + \mu_m^2}} \right] \frac{G_{nm} K_{nm}(x, y)}{\lambda_n^2 + \mu_m^2 - \alpha^2} \right\}, \quad (4)$$

$$\text{where } G_{nm} = 4 \int_0^r e^{-\frac{x^2}{r^2}} \cos \lambda_n x dx \int_0^{\sqrt{r^2 - x^2}} e^{-\frac{y^2}{r^2}} \cos \mu_m y dy, \quad K_{nm}(x, y) = \cos(\lambda_n x) \cos(\mu_m y),$$

$\lambda_n = \pi n / a$, $\mu_m = \pi m / b$, $n, m = 0, 1, \dots, \infty$, $2a$ and $2b$ – the dimensions of an elementary rectangular cell with periodical structure on the solid surface (Fig. 1), $\varepsilon_{nm} = 1$ if $n \neq 0$, $m \neq 0$; $\varepsilon_{nm} = 1/2$ if $n = 0$, or $m = 0$; $\varepsilon_{nm} = 1/4$ if $n = 0, m = 0$.

Every function $K_{nm}(x, y)$ meets the boundary conditions (3). It is held down as much as 49 members in the two-fold series. An attenuation coefficient in the Gaussian beam of about 0.15 1/m is accepted. All the calculations are realized in dimensionless coordinates.

As would be expected, it follows from the results presented that while retreating from the solid surface the temperature in the layers decreases because of diminishing the beam radiation intensity. Along with it, a temperature distribution with respect to the coordinates retains its form (conformity). The temperature value depends substantially on the beam radius, and this dependence is not a linear one. Herewith, for instance, at $z = 1$, that is near the surface, the temperature T^* in the beam centre changes from 0.371 to 0.0556 for the biggest ($r = 1.0$) and the smallest ($r = 0.2$) beam radii, respectively.

Graphic representation of a heat penetration in the solid is illustrated by curve of the type shown in Fig. 3. It must be emphasized that the dependence differs from purely exponential character in the beam. The results represented give evidence of high effectiveness of the approach elaborated. With its help, the depth of heating can be evaluated in connection to the laser radiation source parameters.

Conclusion

The results presented show a high effectiveness of the elaborated approach. With its use, the depth of heating can be evaluated in connection to the laser radiation source. The results obtained are qualitatively consistent with the published experimental data, e.g. those in [21].

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ТЕПЛОВА ІСТОРІЯ ПРИ ЛАЗЕРНОМУ НАГРІВІ ПОВЕРХНІ ТВЕРДОГО ТІЛА

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За допомогою кінцевого інтегрального перетворення по декартових координатах в площині поверхні отримано аналітичний вираз для розподілу температури $T(x,y,z)$ в зразку, що займає напівпростір $z < 0$. Проведені чисельні розрахунки показали, що в більш глибоких шарах значення температури досягається пізніше, ніж на поверхні, оскільки нижніх шарів теплова хвиля досягає пізніше. Швидкість охолодження нижніх шарів менша, ніж верхніх. Крім того, чисельні розрахунки показали, що максимальна температура на заданій глибині слабо залежить від форми розподілу інтенсивності в лазерному пучку. Отримані результати якісно співпадають з експериментальними даними.

ТЕПЛОВАЯ ИСТОРИЯ ПРИ ЛАЗЕРНОМ НАГРЕВЕ ПОВЕРХНОСТИ ТВЕРДОГО ТЕЛА

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С помощью конечного интегрального преобразования по декартовым координатам в плоскости поверхности получено аналитическое выражение для распределения температуры $T(x,y,z)$ в образце, занимающем полупространство $z < 0$. Проведенные численные расчеты показали, что в более глубоких слоях максимальное значение температуры достигается позже, чем на поверхности, поскольку в нижние слои тепловая волна доходит позже. Скорость охлаждения верхних слоев оказывается больше, чем нижних, однако время охлаждения нижних слоев меньше, чем верхних. Кроме того, численные расчеты показали, что максимальная температура на заданной глубине слабо зависит от формы распределения интенсивности в лазерном пучке. Полученные результаты качественно совпадают с экспериментальными данными.