Computer Modeling of the Obtaining Nanostructures Process under the Action of Laser Radiation on Steel

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Abstract. The conditions for the formation of nanostructures in the surface layer of steels with different carbon content (steel 20, 40, 45, 40Cr, U8 and U12), which determine the required temperature (500-1500 K) and the rate of increase (more than 10^7 K/s). The zones of formation of nanostructures depending on the heat flux density on the time of action of the ionizing radiation are determined. It is shown that it is necessary to take into account the rate of temperature rise and the probability of thermoelastic destruction due to the action of temperature stresses. In low speed temperature rise formed micro and submicrostructure that has been confirmed experimentally.

Keywords: nanostructure, submicrostructure, technological parameters, steel, pulse laser radiation

1 Introduction

Nanostructured surface layers can significantly improve the performance of parts by increasing the microhardness of the surface, reducing the modulus of elasticity with increasing yield strength and toughness, which allows you to create on the details of the surface layers to increase the life of the parts working under shock loads and guarantee their long-term strength.

As our reviews presented in [1-5] showed, despite the fact that nanostructures were experimentally obtained under the action of ionizing radiation, the theoretical consideration of the possibility of obtaining nanostructures was not considered. All this is due to the fact that the criteria for obtaining nanostructures (NS) were not formulated, which are formed only in the temperature range 500-1500 K at a temperature rise rate of more than 10^7 K/s, and are intensified by the action of non-stationary temperature stresses of the order 10^8-10^{10} Pa. In addition, the time of action of temperatures should be such that the process of grain size growth under the prolonged action of temperature is not realized. Then these criteria can be expanded to the following: time of cooling to temperatures close to 500 K was not more than $e\cdot\tau_u$ (τ_u – the duration of the radiation pulse) that will ensure the stability of the formation of the NS.

2 Effect of laser radiation on structural materials

2.1 Features of the description of the heat source under the action of the laser on opaque materials

For technological purposes, a focused source of coherent radiation is used, the heat flux density of which is distributed in the focal plane as follows:

$$q\left(r\right)=q_0\left[\frac{2I_1\left(Br\right)}{\left(Br\right)^2}\right]^2 \tag{1}$$

where $I_1(Br)$ is a Bessel function of the first kind of the first order;

$$B=I_1D/\lambda F\,. \tag{2}$$

Where D is the diameter of the lens; λ – wavelength radiation; F – focal length; q_0- – intensity in the center of the spot, calculated by the formula:

$$q_0=\frac{I_1D^2}{4\lambda^2F^2}P_0 \tag{3}$$

where P_0 is the radiation power absorbed by the material.

The heat flux density can be obtained from the product of a time-dependent function and a surface coordinate function:

$$q_n(r\tau)=A\varphi\left(\tau\right)q\left(r\right). \tag{4}$$

Where A is the absorption capacity of the processed material, which generally depends on both the state of the surface (degree of processing, roughness) and its temperature; $q(r)$ – the spatial distribution of the radiation power calculated by the formula (1) taking into account (2) and (3); $\varphi(\tau)$ – describes the time structure of the pulse; for example, for a laser pulse operating in a beam mode with ordered generation, the function can be represented as:

$$\varphi\left(\tau\right)=\left(1-\cos\omega\tau\right). \tag{5}$$

For envelope of lumps the expression is true:

$$\varphi(\tau) = \tau^n \exp(br^m)\ , \tag{6}$$

where n and m are some numbers (integer or fractional).

Modulation of the q-switched laser allows to monoimpulse radiation duration $\approx 10^{-8}$ s, is a temporary structure which can be described by a function that is close to triangular and the slope front may be different from the rear.

The light flux falling on the surface of the material is partially reflected, and the rest of it passes inside the body volume and is absorbed. Inside and on the surface of the body is the heat source distributed in space and time.

The density of the absorbed heat flux for almost all technological applications of the laser varies within the volume of the material according to the Booger law:

$$q_V(z) = q_{V_0}(1-R)e^{-az}\ , \tag{7}$$

where $q_V(z)$, q_{V0} are, respectively, the volume densities of the heat flux of radiation at a distance z and on the surface, W/cm^3,

$$q_{V_0} = \frac{q_n(r,\tau)}{0{,}1\delta}\ . \tag{8}$$

Where $\delta \approx 10^{-4}\ldots10^{-5}$ m – layer, where the light flux is absorbed in the interaction with the conduction electrons; R and α are respectively the reflectivity and light absorption coefficient.

2.2 Model of the interaction of the light beam fluxes and construction materials

Subject to the volume and source of radiation, the amount of probability density is calculated according to the expression (7) with (8), and the surface heat source with heat density of current according to the expression (4) with (5), (6), solve the equation.

Heat balance in the unit volume of the part

The heat balance is represented in the expression:

$$\begin{aligned}
&C[T]\gamma[T]\frac{dT(x,y,z,t)}{dt}+C[T]\gamma[T]\frac{\partial T(x,y,z,t)}{\partial y}V_n+C[T]\gamma[T]\tau_p\frac{d^2T(x,y,z,t)}{dt^2}=\\
&=\nabla\lambda[T]\nabla T(x,y,z,t)+C[T]\gamma[T]V_{\text{тм}}\frac{\partial T(x,y,z,t)}{\partial x}-AL_{\text{ПЛ}}\gamma[T]\frac{dV_{\text{пл}}}{dt}+\\
&+B\frac{q_n(r,\tau)}{0.1\delta}\pm D\frac{dW(x,y,z,t)}{dt}\pm m_aC_a[T_a]\frac{dn_a}{dt}\left(T_a-T(x,y,z,t)\right)\pm\\
&\pm P_{T.X.P}\left(n_A,n_B,T,t_{e,}\right)\frac{dn_{A(B)}}{dt}L_{T.X.P}+q_v(z),
\end{aligned}\tag{9}$$

where $C[T]$ and $\gamma[T]$ is the specific heat and density of the target material corresponding to a temperature T; τ_p is the relaxation time temperature by one Kelvin; V_n is the velocity of the plasma flow of laser radiation or the target relative to it;; $L_{ПЛ}$ and $L_{T.X.P}$ are specific heat of fusion and thermochemical reaction; $V_ф[T]$ – the displacement speed of the evaporation front; $V_{пл}$ – the volume of molten metal; $W(x, y, z, t)$ – energy of deformation of a unit volume target; m_a – mass of the diffusing atom; $Ca[Ta]$ is the heat capacity of the diffusing material at a temperature T_a; $P_{T.X}(n_A, n_B, T, t_{B3})$ – the probability of thermochemical reactions that depend on concentration of the reagents; n_A and n_B, are the temperature T and the time of interaction; t_{B3}; n_A and n_B are the concentration of the reactants that determine the possibility of a reaction.

The amount change of heat in a unit volume (the first term in the left part of the equation) is realized by moving the laser radiation flow along the treated surface or moving the target relative to the laser radiation flow at the rate of V_n (the second term); thermophysical processes: effects on the heat transfer of the final rate of heat propagation (the third term), thermal conductivity(the first term on the right), displacement of the evaporation front(the second term), melting (the third term); collision processes: volumetric heat source due to the action of laser radiation (the fourth term), thermoelastic, thermoplastic and thermo-fatigue processes that determine the energy of deformation of the material of elementary volume (the fifth term); diffusion processes that determine the heat transfer of the diffusing material (the sixth term); thermochemical processes associated with the implementation of chemical reactions between the part material and the coating material or between the components of alloys and composite materials, the volumetric heat source due to the action of the light-beam flow.

When evaporating from a layer of molten metal (Poole-Frenkel conduction mechanism [6, 7]), the evaporation rate is determined by the formula

$$V_ф = V_0 \exp\left(\frac{T^*}{T(0, x, y, z, t)} \right) \tag{10}$$

where V_o and T^* are critical evaporation rates and surface temperatures [8].

To determine these values, we use the approximation of the graphs of the dependence of V_o and T^* on the heat flux density q. For a good approximation, a quadratic function is suitable, the coefficients of which can be determined by the program of approximation of the function with a power basis by the least squares' method. On the charts, the values of q and V_o are indicated on a logarithmic scale, so use the following substitutions:

$$V_0 = 10^{z-3}; \quad q = 10^{s+8}; \;\Rightarrow\; S = \lg q - 8 \tag{11}$$

The value of the heat flux density q can be determined by the formula (2).

V_o and T^* dependences on q through auxiliary variables have the following form:

$$Z = \left(nS^2 + kS + p\right)\cdot 10^{-1};$$
$$T^* = \left(mS^2 + rS + f\right)\cdot 10^{-2}. \tag{12}$$

The coefficients in the formulas (18) for different materials are given in Table. 1.

Table 1. Coefficients *n, k, p, m, r, f* in the formula (18)

Material	*n*	*k*	*p*	*m*	*r*	*f*
Al	1.619	3.0952	8.8571	1.4048	2.5833	3.2321
W	1.7143	10.2857	9.9997	3.2857	3.4428	1.8032
Fe	1.751	3.2502	10.5021	3.2849	-1.9286	37.942
Mo	0.8928	4.7321	10.9731	4.5357	-1.6752	53.652
Cu	-0.0858	1.1319	1.0605	0.8451	3.9713	19.116

The third term on the right of the formula (9) takes into account the change in the amount of heat during melting and is calculated for the volume of the $V_{пл}$ material in which the calculated temperature exceeds the melting point. The specific heat of fusion $L_{пл}$ can be calculated according to the formula:

$$L_{пл} = nT_{пл} f\left(T_{пл}\right)\cdot 4186.8 \tag{13}$$

where n is the number of atoms in the molecule; $f(T_{пл})$ is a function of the dependence of $L_{пл}$ on $T_{пл}$, which can be approximated as a linear dependence of the form:

$$f(T_{пл}) = (1.57T_{пл} + 1428)\cdot 10^{-3} \tag{14}$$

For example, for iron $f(T_{пл}) = 3.5$ cal/g. The specific melting heat $L_{пл}$ in the formula (12) is measured in calories per gram.

The fourth term of the formula (9) calculates the change in the amount of heat due to the action of laser radiation as a volumetric heat source.

The fifth term of the formula (9) takes into account the energy expended on the deformation of the body during the action of the heat source t_u, and the energy returned to the material during stress relaxation (for a time greater than t_u and less than $t_u + \tau_p$).

The deformation energy of a single volume is determined by the formula:

$$W = G\begin{bmatrix} \varepsilon_{xx}{}^2 + \varepsilon_{yy}{}^2 + \varepsilon_{zz}{}^2 + 2\left(\varepsilon_{xy}{}^2 + \varepsilon_{yz}{}^2 + \varepsilon_{zx}{}^2\right) + \\ + \dfrac{\mu}{1-\mu}\ell^2 - \dfrac{2(1+\mu)\alpha_1}{1-2\mu}\ell\left(T(x,y,z,t) - T\right) \end{bmatrix} \tag{15}$$

where $2\varepsilon_{ik} = 2\varepsilon_{ki} = \dfrac{\partial u_k}{\partial i} + \dfrac{\partial u_i}{\partial k}$ *(k, i = x, y, z);* $\ell = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$; ε_{xx}, ε_{yy}, ε_{zz} - e – elongation; ε_{xy}, ε_{yz}, ε_{zx} – shifts relative to the corresponding axes; u_x, u_y, u_z – displacements relative to the corresponding axes; α_l – coefficient of linear expansion of the target material; μ is the Poisson's ratio (the ratio of lateral strain to longitudinal value

μ concluded between 0.1 and 0.5), G is the shear modulus (modulus of the second kind) (for the iron $G = 3{,}5\ldots10{,}3\cdot10^{10}$ N/m^2, $\mu = 0.23\ldots0.31$); $T_н$ – the initial temperature.

Deformations of shifts of ε_{ik} cannot be set arbitrarily, they are connected by differential relations-compatibility conditions [9].

$$\begin{aligned}
&\frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = 2\frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y}; \quad \frac{\partial^2 \varepsilon_{xx}}{\partial y \partial z} = \frac{\partial}{\partial x}\left[-\frac{\partial \varepsilon_{yz}}{\partial x} + \frac{\partial \varepsilon_{zx}}{\partial y} + \frac{\partial \varepsilon_{xy}}{\partial z}\right];\\
&\frac{\partial^2 \varepsilon_{yy}}{\partial z^2} + \frac{\partial^2 \varepsilon_{zz}}{\partial y^2} = 2\frac{\partial^2 \varepsilon_{xy}}{\partial z \partial y}; \quad \frac{\partial^2 \varepsilon_{yy}}{xy \partial z} = \frac{\partial}{\partial y}\left[-\frac{\partial \varepsilon_{zx}}{\partial y} + \frac{\partial \varepsilon_{xy}}{\partial z} + \frac{\partial \varepsilon_{yz}}{\partial x}\right]; \qquad (16)\\
&\frac{\partial^2 \varepsilon_{xx}}{\partial z^2} + \frac{\partial^2 \varepsilon_{zz}}{\partial x^2} = 2\frac{\partial^2 \varepsilon_{zx}}{xz}; \quad \frac{\partial^2 \varepsilon_{zz}}{\partial y \partial x} = \frac{\partial}{\partial z}\left[-\frac{\partial \varepsilon_{yx}}{\partial z} + \frac{\partial \varepsilon_{yz}}{\partial x} + \frac{\partial \varepsilon_{xz}}{\partial y}\right].
\end{aligned}$$

These conditions verify the correct definition of elongation and shear, and their adjustment-the input of additional stresses. To determine the elongation ε_{xx}, ε_{yy}, ε_{zz} and shifts ε_{xy}, ε_{yz}, ε_{zx} use the expression of the thermoelastic displacement potential Φ:

$$\Delta\Phi - \frac{1-2\mu}{2(1-\mu)}\frac{\gamma}{G}\frac{\partial^2\Phi}{\partial t^2} = \frac{1+\mu}{1-\mu}\alpha_1\left[T(x,\ y,\ z,\ t) - T_H\right] \qquad (17)$$

where γ is the density of the part material.

Given that the solution of the problem is carried out in a mobile coordinate system and when entering a stationary or close to it, the second term in the left part of the equation (17) becomes insignificant, we obtain:

$$\Delta\Phi = \frac{1+\mu}{1-\mu}\alpha_1\left[T(x,y,z,t) - T_H\right] \qquad (18)$$

The magnitude of the thermoelastic potential of displacements and the known ratios to find the magnitude of the elongation and changes [10-11].

$$\varepsilon_{ik} = \frac{\partial^2 \Phi}{\partial i \partial k}, \quad (i,k = x,\ y,\ z) \qquad (19)$$

The values of temperature stresses are determined by the expression

$$\sigma_{ik} = 2G\left(\frac{\partial^2\Phi}{\partial i \partial k} - \Delta\Phi \cdot \delta_{ik}\right), \qquad (20)$$

where δ_{ik} is subject to the conditions: $\delta_{ik} = 0$ at $i \neq k$ $(i,k = x,y,z)$; $\delta_{ik} = 1$ at $i = k$.

In the seventh term of the formula (9), taking into account the heat transfer of the diffusing material, the mass of the diffusing atom is determined by the formula.

$$m_a = Mm_p \tag{21}$$

where M is the atomic weight of the applied material; m_p is the mass of the proton.

The change in the concentration of diffusing atoms per unit time can be determined by the expressions:

- at *at* $t < t_k$:

$$\frac{dn_a}{dt} = \frac{j_a}{ez\sqrt{\alpha\tau}}$$

- at *at* $t \geq t_k$:

$$\frac{dn_a}{dt} = \frac{j}{ezL_D}\,, \tag{22}$$

where j is the current density of the introduced atoms; e is the electron charge; z – the charge number of the applied material; L_D – the thickness of the part; t_k – time for which the part will warm up to the entire thickness, $t_k = \frac{L_D^2}{\alpha}$; α is the thermal diffusivity.

The diffusion coefficient is calculated:

$$K_{диф} = a_d d_э^2 V_0 \exp\left(-U/(kT)\right) \tag{23}$$

where a_d is a multiplier of the order of 0.1, determined by the type of crystal lattice; $d_э$ is the distance between the nearest equivalent positions of vacancies in the crystal; V_0 is the value of the order of the frequency of atomic oscillations in the crystal ($10^{12}...10^{14}$ s^{-1}); U is the potential barrier that must be overcome by vacancies when displaced to the neighboring position; k is the Boltzmann constant; T is the absolute temperature.

The eighth term of the formula (9) takes into account the influence of chemical processes on the heat balance in the target. In the interaction of laser radiation with substances consisting of polyatomic molecules, a whole cycle of chemical transformations is possible, such as the excitation of a molecule with its subsequent dissociation (decomposition) into active particles (ions); rearrangement of atoms in the structure of the molecule; movement of individual atoms from one part of the molecule configuration to another; accession to the excited molecule of another molecule; transfer of excitation energy from one molecule to another; capture electrons to form negative ions; recombination of an ion with an electron or an ion with a molecule. The concentration of chemical transformations in the first approximation is directly proportional to the density of the absorbed energy and the chemical yield (the average number of chemical transformations in the absorption of single energy). As a result of chemical reactions between ions and radicals of the plasma-forming gas and atoms of the material, it is possible to remove the material in the form of volatile compounds, which is used in plasma chemical etching (for example, adding 10 % oxygen to argon can increase the rate of removal of the material due to chemical reactions by 10-15 times). The rate of plasma-chemical etching is 2…10 nm/s. In the processing of elements W, Te, Mo, Ta fluorine-containing gases are formed volatile fluoride, and Al in the processing of chlorine-containing gases – volatile chlorides. Thermo- and plasma-chemical reactions can also contribute to an increase in the mass and volume of the workpiece due to the formation of chemical compounds with the reaction gas. Laser irradiation in the atmosphere of a chemically active gas or in a mixture of inert and chemically active gases, such as O_2, Ar $^{+}$ N_2, Ar $^{+}$ N_2, etc., is accompanied by the following processes that ensure the growth of the film of the chemical compound: the reaction between the chemically active ions A and the atoms of the target B, followed by the transfer of AB molecules to the substrate; reaction between atoms and ions of the chemically active gas A, A^+, A^- and atoms of the coating; reaction between atoms and ions A, A^+, A^- and sprayed particles B in the gas phase, followed by the deposition of molecules AB on the surface of the target.

In the case where a multicomponent substance AB (chemical compound, alloy) is exposed to laser irradiation, the ratio of surface concentrations in the established process will be as follows:

$$\frac{n_A(0)}{n_B(0)} = \frac{n_{A.V}}{n_{B/V}}\left(\frac{M_A}{M_B}\right)^{1/4} \tag{24}$$

where $n_{A,V}$ and $n_{B,V}$ are the concentrations of atoms A and B in the target volume.

The surface layer is enriched with a heavier component.

If the working substance continuously enters the surface and decomposes there under the action of irradiation, then in the simplest case the rate of change in the surface concentration of the molecules of the compound that have entered N_1 and have not entered N_2 will be determined by the equations:

$$\frac{dN_1}{dt} = \frac{N_0 \sigma_p J_e}{e} \tag{25}$$

$$\frac{dN_0}{dt} = n_0 - \frac{N_0}{\tau_0} - \frac{dN_1}{dt} \tag{26}$$

where σ_p is the reaction cross-section depending on the properties of the compound and the energy of laser radiation; n_0 is the number of molecules entering the unit surface area per unit time; τ_0 is the average time during which the unreacted molecules are on the surface before evaporation.

Having integrated the system of equations (20)–(26) in the case of a small flow n_0, we obtain:

$$N_0(t) = n_0\sigma_h\tau_0 J_\ell \left(e+\sigma_h\tau_0 J_\ell\right)^{-1} \tag{27}$$

Here the designation is introduced, $\frac{1}{\tau_1} = \frac{1}{\tau_0} + \frac{\sigma_p J_e}{e}$ and $N_0(t)$ is the initial concentration of molecules at the time of laser irradiation at $t = 0$. After a period of time $t >> \tau_l$ establishes an equilibrium concentration of, equal to $n_0\tau_1$, and for the reaction to proceed with a constant speed:

$$dN_1 / dt = n_0\sigma_p\tau_0 J_e \left(e+\sigma_p\tau_0 J_\ell\right)^{-1} \tag{28}$$

In general, this rate depends on all the parameters of the process $\left(E_e,\ J_\ell,\ T,\ n_0\right)$, but if the reaction is carried out at sufficiently low T and high J_ℓ, so that $\sigma_p\tau_0 J_\ell >> 1$ the reaction rate is determined only by the rate of adsorption and for a small value of n_0 is not very high.

At high flux density n_0, sufficient to create a thicker coating than a monolayer, the reaction rate is determined only by the irradiation regime and is independent of n_0 and T:

$$dN_1 / dt = N_0\sigma_p J_\ell / e \text{ at } n_0\tau_1 >> N_0 \tag{29}$$

3 The heat transfer on the surface of the part

Heat flow on the target surface is created by the following factors:

- collision processes: heat released on the surface due to the action of laser radiation (the first term on the right), the heat flux withdrawn from the thermoelectrons (the second term), and secondary photons (the third term);
- thermophysical processes: removal of heat flow with evaporated material (fourth term), the material in the liquid phase, if the conditions for its release (fifth term), thermal radiation of the heated surface (sixth term) and condensed atoms, previously evaporated (seventh term);
- plasma chemical processes, realized by the reactions of the laser radiation flux with the evaporated material of the part or adsorbed gases (eighth term); this energy is transmitted by radiation.

The energy transfer is also carried out by the radiation of the laser radiation quantum flux (the last term):

$$\begin{gathered}-\lambda[T]\frac{\partial T(x,\ y,\ z,\ t)}{\partial x} = F_{\ell,r} - F_{тэ} - F_{эф} - F_{исп} - F_{т} - \sigma\varepsilon T^4(0,\ y,\ z,\ t) \pm \\ \pm F_{конд} + F_{пх} + \sigma\varepsilon_c T_c^4,\end{gathered} \tag{30}$$

where σ is the Stefan-Boltzmann constant; ε and ε_{-} are the degree of blackness of the target surface and the medium; T_c is the temperature of the medium.

Each term is considered in more detail in [3].

Heat flux density due to the action of laser radiation:

$$F_{ли} = \frac{I_i D^2}{4\pi\lambda^2 F^2} P_0 \tag{31}$$

The second term takes into account the removal of heat flow due to the emission of electrons by the heated surface of the target – thermo-electronic emission. The density of the heat flow discharged with electrons,

$$F_{TЭ} = J_Э \phi(T) \tag{32}$$

where $\varphi(T)$ is the work of the electron output, eV, at the surface temperature T; $J_э$ is the density of the emission current, which is determined by the Richardson equation:

$$J_э = \left(1 - \overline{r}\right) A \cdot T^2 \cdot \exp\left(-e\phi_0 / kT\right) \tag{33}$$

Here $\overline{r}$ – the average electron energy reflection coefficient of the potential barrier at the boundary "solid-vacuum", it can reach several percent for pure metals; A – Richardson constant, $A = 4\pi m_e k^2 e/h^3$ =$1,204 \cdot 10^6$ A/ m ^{2}(K)^2; φ_0 – the electron work function at $T = 273$ K; k – is the Boltzmann constant.

For most metals φ lies in the range 4…5 eV.

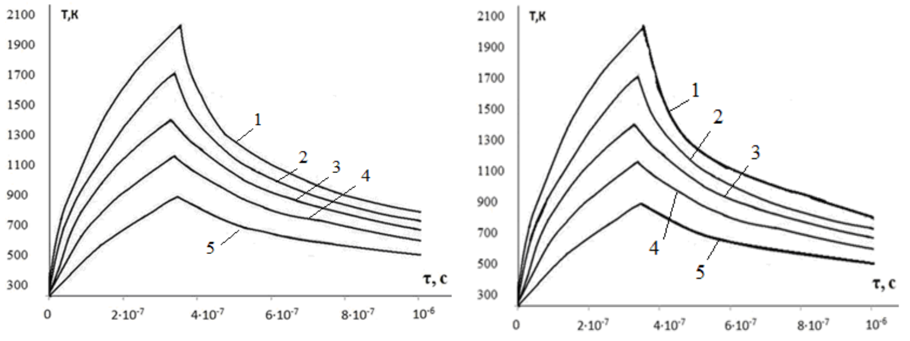
4 Calculation results and discussion

Calculations of temperature fields under the action of laser radiation flow on the part are carried out on a computer by the finite element method. The process of computer simulation is implemented by dividing the equations by coordinates and computer calculations are carried out separately by coordinates, and then the coordinates of the corresponding temperature points are summed. The calculation of temperature stresses is also related to computer simulation, which allowed to divide each step into two half-steps. In the first half-step of the first step, calculations are carried out without taking into account computer modeling, that is, the temperature of the stresses is equal to zero. In the first half-step temperature is calculated on which the second half-step, taking into account the obtained stresses, and hence the deformation energy are adjusted by computer and the temperature stress values in the next step are already obtained temperatures are starting and in the first half-step of the second step (and subsequent) the previous temperature is the initial and the process is repeated by computer.

As a result of the calculations, the temperature fields in the zone of laser radiation on steels during heating and cooling were determined. Calculations were carried out for a wide range of heat flux densities and times of its action, but only those whose maximum temperatures during heating and cooling are close to those necessary for obtaining nanostructures (500-1500 K) and the rate of temperature rise exceeds 10^7 K/s are discussed.

So in Fig. 1 the dependences of the maximum temperature in the spot ($r = 0.1$ mm) under the action of heat fluxes with peak density $q = 3 \cdot 10^{10}$ W/m^2 (1), $q = 2.5 \cdot 10^{10}$ W/m^2 (2); $q = 2 \cdot 10^{10}$ W/m^2 (3); $q = 1.5 \cdot 10^{10}$ W/m^2 (4) and $q = 10^{10}$ W/m^2 (5) with an action time of 10^{-7} s on steel 20 Fig. 1 (a) and steel 40Cr Fig. 1 (b). It can be seen that for the first two modes, the maximum temperatures on steel are 20 (Fig. 1 *a*) exceed the temperature of 1500 K, but the time for which they operate $2.1 \cdot 10^{-7}$ s for the first mode and $1.1 \cdot 10^{-7}$ s for the second during this time, the relaxation of the temperature field will not lead to a significant increase in the initial grain size so that not only in 3, 4 and 5 modes should be expected to obtain nanostructures but in the first and second modes. For heating and cooling modes, the rate of temperature rises and fall exceeds 10^7 K, which confirms the probability of nanostructures formation.

For steel 40Cr times in which the temperature exceeds 1500 K for the first mode is $1.7 \cdot 10^{-7}$, and 10^{-7} with, respectively, for the first and second mode is even less than for steel 20 and in this case, the effect of this temperature on grain growth is less significant. The results of similar calculations for steel 40 and 45 are shown in Fig. 2.

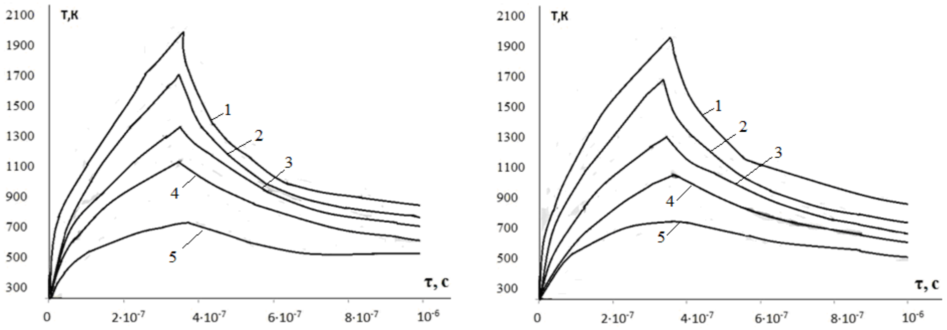


a *b*

Fig. 1. Temperature at a depth of 1 μm under the action of laser radiation, the peak heat flux density is $3 \cdot 10^{10}$ W/m^2 (1), $2.5 \cdot 10^{10}$ W / m^2 (2), $2 \cdot 10^{10}$ W/m^2 (3), $1.5 \cdot 10^{10}$ W/m^2 (4) and 10 W/m^2 (5) for steel 20 (*a*) and steel 40Cr (*b*), operating at the initial time $3 \cdot 10^{-7}$ s

In this case, the values of the maximum temperatures are reduced and amount to values of the order of 1900 K, whereas they exceed 2000 K for steel 20, the nature of the change in the maximum temperature over time has been preserved, the temperature growth rate for these materials exceeds 10^7 K/s, which suggests that for these materials there is a real possibility of obtaining nanostructures.

For high-carbon steels U8 and U12 under the action of thermal $3 \cdot 10^{10}$ W/m^2 and $2.5 \cdot 10^{10}$ W/m^2 maximum temperatures also exceed 1500 K and are close to 2000 K, but the time of action of these temperatures does not exceed $2 \cdot 10^7$ s, for these materials for other modes up to the time of action 10^{-6} s temperature mode promotes the formation of nanostructures and the rate of temperature rise exceeds 10^7 K/s, this confirms that for these materials the probability of formation of nanostructures is high (Fig. 3).

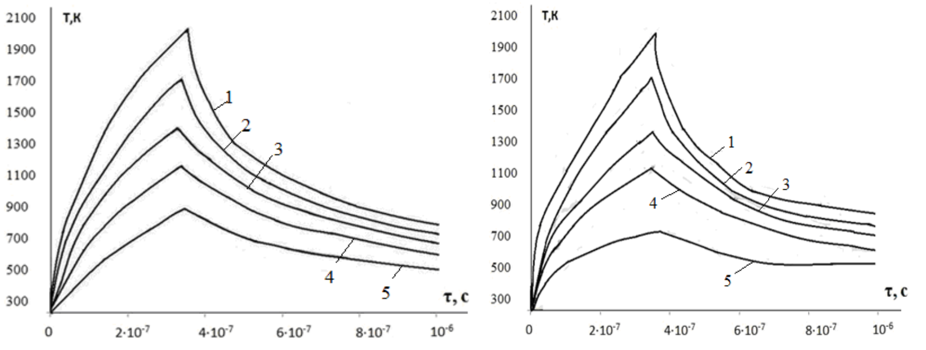


a *b*

Fig. 2. Temperature at a depth of 1 μm under the action of laser radiation, the peak heat flux density is $3 \cdot 10^{10}$ W/m^2 (1), of $2.5 \cdot 10^{10}$ W/m^2 (2), $2 \cdot 10^{10}$ W/m^2 (3), and $1.5 \cdot 10^{10}$ W/m^2 (4) and 10^{10} W/m^2(5) of the steel 40 (*a*) and steel 45 (*b*), the current at the initial moment of time $3 \cdot 10^{-7}$ s

When the temperature increases above 1500 K, the grain size increases and it is impossible to obtain nanostructures.

A wide range of steel grades was studied to obtain a common result and to find modes in which it is impossible to obtain nanostructures.



b

a

Fig. 3. Temperature at a depth of 1 μm under the action of laser radiation, the peak heat flux density is $3 \cdot 10^{10}$ W/m^2 (1), of $2.5 \cdot 10^{10}$ W/m^2 (2), $2 \cdot 10^{10}$ W/m^2 (3), and $1.5 \cdot 10^{10}$ W/m^2 (4) and 10^{10} W/m^2(5) on steel U8 (*a*) U12 (*b*), the current at the initial moment of time $3 \cdot 10^{-7}$ s

To estimate the size of the zone of formation of the nanostructures it is necessary to have the radius of the zone of formation of nanostructures built for this space-time pattern of the temperature distribution along the radius and in time for example, steel 40Cr steel under the action of heat flux with density of $3 \cdot 10^{10}$ W/m^2 when the radius of the spot is 0.1 mm (Fig. 4).

It can be seen that the radius of the temperature decreases compared to the maximum at 200-250 K, which indicates the insignificance of the influence of the zone where the temperature exceeds the permissible (1500 K) on the nature of grain growth, which will be insignificant. All this once again confirms the possibility of obtaining nanostructures in the layer with a depth of about micrometers and a radius of more than 0.1 mm.

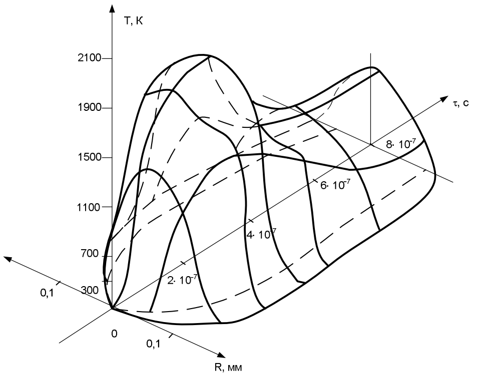


Fig. 4. Spatio-temporal pattern of temperature distribution over a radius in time under the action of laser radiation on steel 40Cr with a heat flux density of $3 \cdot 10^{10}$ W/m^2 at a spot radius of 0.1 mm

Practically the same or similar temperatures can be obtained at heat flux densities two orders of magnitude less than $q = 3 \cdot 10^8$ W/m^2 and its action time $3 \cdot 10^{-3}$ s (Fig. 5), but in this case, nanostructures are not formed, but micro and submicro clusters of 1-3 μm and 0.5-0.8 μm in size are formed [4]. all this confirms the thesis that to obtain nanostructures it is necessary to have temperature growth rates greater than 107 K/s, and in this case the maximum temperature growth rate reaches only $6 \cdot 10^6$ K/s and in this case only submicrostructures can be formed.

To select the technological parameters of laser radiation in the preparation of nanostructures on the basis of calculations of temperatures and rates of their increase, the dependences of the critical densities of heat fluxes $q_{\text{cr max}}$ and $q_{\text{cr min}}$ on the time of their action were constructed, at which nanostructures are formed on steel 40Cr (Fig. 6). The same method can be used to obtain dependencies for other steels.

It is seen that the zone of technological parameters for obtaining nanostructures is limited to direct $q_{\text{cr max}}$, $q_{\text{cr min}}$, the zone where the rate of temperature growth is insufficient and the zone where the high probability of thermoelastic destruction is shown to be possible to choose the technological parameters of laser radiation, the heat flux density and the time of its action, ensuring the production of nanostructures in the surface layer.

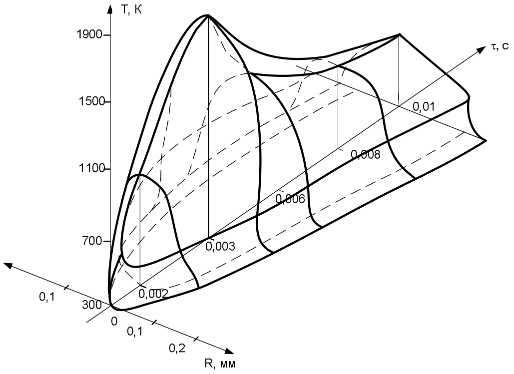


Fig. 5. Spatiotemporal pattern of temperature distribution over radius and time under the action of laser radiation with a heat flux density of $3 \cdot 10^8$ W/m^2 at a spot radius of 0.1 mm

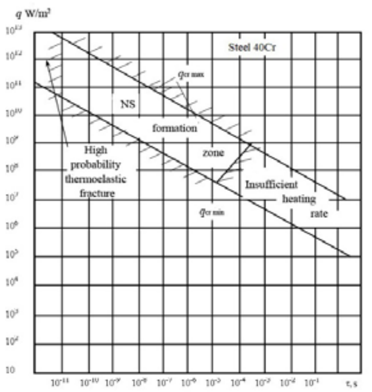


Fig. 6. Dependence of critical values of heat flux densities on the time of their action ensuring the production of nanostructures

5 Conclusions

The conditions for the formation of nanostructures in the surface layer of steels with different carbon content (steel 20, 40, 45, 40Cr, U8 and U12), which determine the required temperature (500-1500 K) and the rate of increase (more than 10^7 K/s). It was found that with an increase in temperature above 1500 K The grain size increases and it is impossible to obtain nanostructures.

The zones of formation of nanostructures depending on the heat flux density on the time of action of the ionizing radiation are determined.

It is shown that it is necessary to take into account the rate of temperature rise and the probability of thermoelastic destruction due to the action of temperature stresses. So with the low speed temperature rise formed micro and submicrostructure that has been confirmed experimentally.

The process of computer simulation is implemented by dividing the equations by coordinates and computer calculations are carried out separately by coordinates, and then the coordinates of the corresponding temperature points are summed. The calculation of temperature stresses is also related to computer simulation, which allowed to divide each step into two half-steps. In the first half-step of the first step, calculations are carried out without taking into account computer modeling, that is, the temperature of the stresses is equal to zero. In the first half-step temperature is calculated on which the second half-step, taking into account the obtained stresses, and hence the deformation energy are adjusted by computer and the temperature stress values in the next step are already obtained temperatures are starting and in the first half-step of the second step (and subsequent) the previous temperature is the initial and the process is repeated by computer. All this confirms that without computer modeling the process could not be realized.

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