The mathematical model for description of the processes of heat-and-mass transfer under the pulsed laser exposure is proposed. It consists of heat and diffusion problems taking into consideration the nonlinear dependence of the carbon diffusion coefficient on temperature and concentration. 

In consequence, we have obtained the distribution of the temperature and concentration fields in the laser exposure range. An explanation of the formation mechanism for the oscillation structure of the carbon concentration distribution in the sample depth is proposed.

Introduction

The problem connected with mass transfer under the action of the pulsed laser exposure is of great importance for the investigation of the diffusion processes which take place in non-equilibrium conditions and it is necessary to take them into account during the analyses of the kinematics of the phase transformation and the following usage for improvement of the mechanical characteristics of the surface layers of steels and alloys [1-5].

The choice of the optimum parameters of the laser exposure, which are different for the definite alloy, is one of the problems, which must be solved in the case of the pulsed laser treatment of the surface to obtain the maximum solubility of carbon in γ-solid solution. Therefore, development and application of the mathematical model, which will help to optimize the values of these parameters is the problem of great importance.

The purpose of the present work is numerical investigation of the temperature and concentration fields in the pulsed laser exposure range and prediction of the optimum parameters of laser treatment.

1. Formulation of the problem and the mathematical model

The proposed mathematical model applied for the calculation of the diffusion redistribution of carbon in austenite explicitly takes into consideration the nonlinear dependence of the diffusion coefficient on temperature and concentration of carbon. It is presented by the one-dimensional Stephan’s problem with one movable boundary [4] and consists of the diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[ D(C,T) \frac{\partial C}{\partial x} \right], \quad (1)$$

of the initial condition

$$C(x,0) = C_0, \quad (2)$$

of the boundary condition on the surface of the sample
and on the movable boundary

\[
D(C, T) \frac{\partial C}{\partial x} \bigg|_{x=\pm(t)} = -C \frac{\partial C}{\partial t},
\]

where \( C_0 \) is the equilibrium concentration of carbon. The dependence of the diffusion coefficient on concentration and temperature has the form

\[
D(C, T) = D_0(C) \exp \left[ -\frac{\Delta H(C)}{RT} \right],
\]

where \( R \) is the universal gas constant.

Using the experimental data \([5]\), we shall write the interpolation dependence of the factor of the diffusion frequency \( D_0(C) \) and the activation energy \( \Delta H(C) \) and the expression for diffusion coefficient

\[
D(C, T) = \left( C^2 - 12.8C + 48.8 \right) \exp \left\{ \frac{0.25C^2 + 4.22C - 154.4}{8314T} \right\}.
\]

The temperature \( T \) is determined with the help of the solution of the one-dimensional heat problem, which consists of the heat-transfer equation

\[
\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2},
\]

where \( a \) is the heat-transfer coefficient of the condition,

\[
T(x,0) = T_0,
\]

where \( T_0 \) is the temperature of the ambient (let’s take \( T_0 = 300K \) ) and two boundary conditions

\[
\lambda \frac{\partial T}{\partial x} \bigg|_{x=h} + \alpha T \bigg|_{x=h} = 0,
\]

\[
\lambda \frac{\partial T}{\partial x} \bigg|_{x=0} = Aq_0 f(t),
\]

where \( \lambda \) is the heat-transfer coefficient, \( \alpha \) is the heat exchange coefficient, \( h \) is the depth of the sample, \( A \) is the absorption coefficient on power, \( q_0 \) is the maximum value of the density of the radiation power, \( f(t) = Bte^{-\gamma t} \) is the time factor proposed in \([6]\).

The diffusion and heat problems are the one-dimensional ones, because the following relation is fulfilled

\[
\frac{r_f^2}{a} \gg \tau,
\]

where \( \tau \) is the duration of the pulse, \( r_f \) is the radius of laser spot.
2. Results of numerical simulation

The numerical solution of the heat problem (7)-(10) was carried out at the following values of the parameters (Table 1).

Table 1. Values of the parameters for the heat problem solution.

<table>
<thead>
<tr>
<th>$A$</th>
<th>$a$, m/s</th>
<th>$\alpha$, W/m$^2$K</th>
<th>$\lambda$, W/m-K</th>
<th>$q_0$, W/m$^2$</th>
<th>$\tau$, ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>0,8</td>
<td>6,84·10$^{-6}$</td>
<td>3·10$^{7}$</td>
<td>42</td>
<td>4,7·10$^{-6}$; 1·10$^{7}$; 4,7·10$^{6}$</td>
<td>4</td>
</tr>
</tbody>
</table>

Different values of the density of the radiation power $q_0$ were used. The following relations [6] were used for $B$ and $\gamma$ parameters

$$\gamma \approx \frac{2,9876}{\tau}, \quad B = \gamma^2 \tau.$$  \hspace{1cm} (12)

Fig. 1. Temperature distribution at $q_0 = 4,7 \cdot 10^7$ Watt/m$^2$.

Fig. 2. Temperature distribution at $q_0 = 10^7$ Watt/m$^2$.

Fig. 3. Temperature distribution at $q_0 = 4,7 \cdot 10^6$ Watt/m$^2$.

Fig. 4. Temperature distribution in depth of the sample for $q_0 = 4,7 \cdot 10^6$ Watt/m$^2$. 
The results of the numerical solution (Figs. 1-3) show that the maximum temperature is reached on the surface of the sample, then it decreases monotonously and tends to the ambient temperature; this does not contradict the experiment and underlines the adequacy of the selected model.

Besides, the increasing of the power density of the laser radiation from $4.7 \cdot 10^6$ $\text{Watt/m}^2$ up to $4.7 \cdot 10^7$ $\text{Watt/m}^2$ results in the temperature increasing in the upper layer of the sample (Figs. 4-6) and in changing of the character of the temperature distribution in depth (the plateau vanishing) for short intervals of time. The time-temperature parameters of the plateau in the case of low power density correlate with the value of the pulse duration.

The disappearance of the plateau (Figs. 4-6) is connected with the energy absorption by the ambient during partial melting. The melting takes place only in the case when $q_0 = 4.7 \cdot 10^7$ $\text{Watt/m}^2$ and starts at the moment $t_0 \approx 5.0 \text{ ms}$.

The proposed mathematical model allows selecting the technological parameters of the laser radiation when the partial melting of the surface takes place, and it allows controlling the depth of the laser exposure zone. It simplifies the solution of the experimental problems of laser treatment of steel and alloys. For the case $q_0 = 4.7 \cdot 10^7$ $\text{Watt/m}^2$ one can determine the dependence of the coordinate of the melting front $\xi(t)$ (and the diffusion front, respectively) and its rate $\xi'(t)$ on time by means of numerical solution of the following equation

$$T(\xi(t), t) = T_m,$$  \hspace{1cm} (13)

where $T_m$ is the temperature of the melting

$$\xi(t) = -0.00022 + (0.04655 - 0.68365t)t,$$  \hspace{1cm} (14)

$$\xi'(t) = \frac{d\xi}{dt} = -1.36730t + 0.04655,$$  \hspace{1cm} (15)
with the help of expression (15) one can estimate the depth of penetration of the concentration front under the action of the pulsed laser radiation from $\xi'(t) = 0$ condition.

Relation (14) helps us to estimate the dimensions of the zone of carbon redistribution and the strength characteristics of the alloy (for example, hardness) by means of the semi-

empirical formula [7]

$$H(C) = 4200\sqrt{C} - 400(C - 0.02).$$  

(16)

Then the results of the solution of the heat problem (7)-(10) were used for the numerical solution of the problem connected with the redistribution of the carbon atoms in the case of laser treatment of the sample surface, (i.e., the diffusion problem (1)-(6)).

The numerical integration took place in the case when the density of the radiation power $q_0 = 4.7 \times 10^7 \text{Watt/m}^2$ was in agreement with the surface partial melting. The experimental maximum solubility of carbon in $\gamma$–solid solution in the case of the pulsed laser treatment is achieved due to the high rate of heating ($10^5$-$10^6$ degree/s), then this state is fixed as a result of the high rate of cooling with the help of the surrounding matrix. Certainly, everybody knows that the maximum rate of heating is reached in the conditions of the partial surface melting. The solution of the diffusion problem in these conditions is very interesting.

The results of the numerical solution of the diffusion problem (Figs. 7) show that the concentration peak is formed in the region of the diffusion front at the moment when the melting starts and then the peak shifts into the sample depth leading the diffusion front.

At a definite moment of time (within $\Delta t = 0.5 \text{ms}$ after beginning of the diffusion front movement) the distribution of the carbon concentration in depth has oscillating structure, that can be interpreted as movement of the nonlinear “wave of the concentration”, which appears due to the nonlinear dependence of the diffusion coefficient on concentration and temperature. In the course of time the amplitude of these oscillations increases. The extent of the oscillations in depth increases too.

One can smooth out this behavior of the concentration distribution by means of introduction of the additional factors, which help to take into consideration the high rate of hardening of the laser exposure zone due to the surrounding cold matrix.

It should be mentioned that the same concentration oscillations were observed in work [8], which was concerned with investigation of the perlite steel. Thus, we propose the
diffusion model with Stephan’s boundary condition, which is considered to be nonlinear due to the dependence of the diffusion coefficient on concentration and temperature. The problem of the temperature distribution in the sample for different values of the laser radiation power density has been solved. This model is applied for description of carbon redistribution in $\gamma$–solid solution in the zone of pulsed laser exposure of the austenitic steel.

Conclusions

The present model allows selecting the technological parameters of the laser radiation, which help to obtain partial melting of the surface. It allows controlling the depth of the laser exposure zone and estimating the dimension of the carbon redistribution zone and the strength characteristics. The numerical calculations show that the carbon concentration distribution in depth of the sample has the oscillation structure that can be interpreted as movement of the nonlinear wave of the concentration, which appears as a result of the accumulation of the nonlinear effects due to the concentration dependence of the diffusion coefficient.

The given model may be applied for investigation of the diffusion of other elements in steel and alloys, the diffusion coefficients of which are comparable with the diffusion coefficient of carbon; it may be also used in the case of surface scanning by laser beam.

References