Mathematical model of thermal processes in metals during pulse processing with concentrated energy fluxes

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Abstract. The paper considers mathematical modeling of thermal processes in metals during pulsed processing by concentrated energy flows. Calculations of thermal processes in steels under pulsed heating are given, considering the phase transformations and the temperature dependences of the thermophysical properties, as well as the space-time characteristics of the thermal energy source. It is shown that the created mathematical model is universal for various sources of thermal energy and adequately describes the space-time distribution of temperature fields during pulsed heating of the surface layers of metals and alloys.

1. Introduction

When designing modern technologies for modifying the structure and properties of metal products, a combination of computer modeling of processes in metal and experimental verification of the agreement between calculations and real structure formation is traditionally used. Moreover, computer modeling is the first stage, the second is the assessment of the modes of exposure to the material by means of experimental verification. The combination of these two stages makes it possible to solve the problem of improving the operational characteristics of machine parts and tools. The operational properties of metal products largely depend on the modes of heat treatment.

One of the most effective ways to obtain high performance properties is thermal cycling treatment. [1]. A promising direction for improving thermal cycling treatment is the use of periodic pulsed short-term heating of the surface layer of metals and alloys, in particular steels. [2, 3]. Pulse heating has a number of advantages over traditional methods: reduced processing time, high energy efficiency, and obtaining surface nanometric layers. For pulsed heating, concentrated energy fluxes can be used, such as laser radiation, electron beams, plasma jets, high-frequency heating, etc. [4]

The use of concentrated energy fluxes makes it possible to carry out pulsed heating of the surface layers at a rate of tens to millions of degrees per second and to provide a cooling rate of the surface layer practically up to 10⁶ K/sec. Such a high-speed pulsed action, as shown in the works, makes it possible to obtain highly dispersed structures up to nanometric and to form amorphous surface layers. Consequently, for the development of technologies for surface modification of structure and properties using pulsed heating, it is necessary to mathematical modeling of thermal fields, the kinetics of structure formation, and thermomechanical stresses in the heat-affected zone of the energy source under substantially non-stationary conditions. The modeling task can be broken down into three stages. At the first stage, thermal fields are simulated taking into account the dependence of the
thermophysical characteristics of the metal being processed, the dependence of the density of energy 
release over the volume of the processed material. The second stage is the calculation of the arising 
internal stresses during pulsed heating and cooling, considering the calculation of the temperature 
fIELDS according to the first stage. The third stage consists in modeling the kinetics of phase transitions 
and structure formation under pulsed action by a source of thermal energy. For most cases, in the 
development of surface hardening technologies, one can restrict oneself to modeling the first stage.

The purpose of this work is to describe the thermal fields in steels during pulsed heating, taking 
into account phase transformations and the dependences of thermophysical properties on temperature, 
as well as the space-time characteristics of the thermal energy source.

To describe thermal processes, mathematical modeling of heating and cooling of the processed 
material is used, taking into account the space-time distributions of temperature fields and the 
properties of the processed material. The mathematical model is based on the numerical solution of the 
non-stationary heat conduction equation:

\[ c(T) \cdot \rho(T) \frac{dT}{dt} = \text{div} [\lambda(T) \cdot \text{grad}T] - \rho L \frac{d\phi}{dt} + Q_v(x, y, z, \tau), \tag{1} \]

\(c(T)\) – heat capacity of material,
\(\rho(T)\) – density of material,
\(\lambda(T)\) – thermal conductivity of material,
\(T\) – temperature,
\(\tau\) – duration,
\(L\) – heat of melting,
\(\phi\) – fraction of liquid phase in a volume element,
\(Q_v\) – function describing the space-time energy release in a material.

It is assumed that the workpiece is a plate, the spatial dimensions of which significantly exceed the 
heat-affected zone of the heat source. If it is necessary to take into account the dimensions of the 
workpiece to be processed, this is done by setting conditions at the boundaries of the computational 
domain. In many practical cases, it is possible to switch from a 3D problem to a 2D or 1D problem. 
With a source of thermal energy rapidly moving over the surface, for example, an electron beam, the 
two-dimensional formulation of the problem is legitimate. If the spatial dimensions of the energy 
source on the surface significantly exceed the dimensions of the heat-affected zone deep into the 
product, then the solution of the one-dimensional heat conduction equation can be used, since heat 
transfer occurs only inside the plate [5].

2. Experiment

The diagram of the computational domain and the coordinate system are shown in the figure 1. 
Computational domain: X-axis - 2A, Y-axis - 2B, and Z-axis – C.

![Figure 1. Scheme of surface treatment with a thermal energy source.](image)

Initial condition: 
\[ T(x, y, z, 0) = \text{const} = T_0. \tag{2} \]

Border conditions:
\[
\frac{\partial T}{\partial x} |_{x=0} = \frac{\partial T}{\partial y} |_{y=0} = 0, 
\]
(3)

\[
\frac{\partial T}{\partial x} |_{x=A} = \frac{\partial T}{\partial x} |_{x=A-\delta x}, 
\]
(4)

\[
\frac{\partial T}{\partial y} |_{y=B} = \frac{\partial T}{\partial y} |_{y=B-\delta y}, 
\]
(5)

\[
\frac{\partial T}{\partial z} |_{y=C} = \frac{\partial T}{\partial z} |_{y=C-\delta z}. 
\]
(6)

Boundary conditions on the surface of the computational domain:

\[
-\lambda \frac{\partial T(x,y,0,t)}{\partial z} = \alpha (T(x,y,0,t) - T_1) 
\]
(7)

\(T(x,y,0,t)\) – surface temperature,
\(T_1\) – medium temperature,
\(\alpha\) – heat transfer coefficient.

With traditional substitution \(\frac{\partial \psi}{\partial t} = \frac{\partial T}{\partial t} \cdot \frac{\partial T}{\partial \psi}\) we bring the equation (1) to the form

\[
\varepsilon E \rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} (\lambda \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (\lambda \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (\lambda \frac{\partial T}{\partial z}) + Q_v(x,y,z,t), 
\]
(8)

\(\varepsilon\) – effective heat capacity.

The thermophysical properties of the metal were taken in the form [6]:

\[
c_E = \begin{cases} 
  c_S(T), & T \leq T^* \\
  \frac{c_S(T) + \varepsilon_L \frac{\partial \psi}{\partial T}}{2}, & T^* < T \leq T_L, \\
  c_L, & T > T_L 
\end{cases} 
\]
(9)

\[
\lambda = \begin{cases} 
  \lambda_S(T), & T \leq T^* \\
  \lambda^* (1 - \psi) + \lambda_L \psi, & T^* < T \leq T_L \\
  \lambda_L, & T > T_L 
\end{cases} 
\]
(10)

\[
\rho = \begin{cases} 
  \rho_S(T), & T \leq T^* \\
  \rho_S(1 - \psi) + \rho_L \psi, & T^* < T \leq T_L \\
  \rho_L, & T > T_L 
\end{cases} 
\]
(11)

Here the indices S and L refer to the solid and liquid phases, respectively. We write the function of the liquid phase fraction on temperature using the example of iron-carbon alloys in accordance with the theory of a quasi-equilibrium two-phase zone [7].

\[
\psi = \left[ \frac{T_A - T}{T_A - T_L} \right]^{1/k}, 
\]
(12)

\(T_A\) – melting point of pure ferrum;
\(T_L\) – liquidus temperature;
\(k\) – carbon distribution coefficient.

According to [7], the temperature \(T^*\) corresponds to the fraction of the liquid phase \(\psi = 0.05\), taken as the beginning of the two-phase zone.

With laser radiation, heating occurs superficially (since the penetration depth with laser radiation is less than 1 \(\mu m\), and the depth of the heat-affected zone is much greater). When using an electron beam, high-frequency currents and heating by electric current, the distribution of energy release both in depth and over the surface, that is, the energy release depends on the depth of heating, which means that volumetric heating of the surface layer occurs.

Equation (8) can be simplified using the Kirchhoff transformations [8] and introducing the enthalpy \(H\) and the conversion temperature \(F\)
\[ H = \int_{T_0}^{T} \rho C_E \, dt \] (13)

\[ F = \frac{1}{\lambda} \int_{T_0}^{T} \lambda \, dt, \] (14)

\( T_0 \) – base temperature,
\( \lambda_0 \) – thermal conductivity coefficient at base temperature.

Considering (14), equation (8) is transformed to the form

\[ \frac{\partial H}{\partial \tau} = \lambda_0 \left( \frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} + \frac{\partial^2 F}{\partial z^2} \right) + Q(x, y, z, \tau) \] (15)

In the numerical solution of equation (15), an explicit finite-difference method was used. The solution is implemented as a program in C++.

3. Results
To check and calibrate the program, we calculated the distribution of thermal fields in the surface layer of a U8 steel plate treated with a relativistic electron beam with energy. Samples were provided by the Department of Physical Metallurgy of the Lipetsk State Technical University. The compared experimental and calculated data agree within the error limits.

For clarity, the figures below show the results of one-dimensional calculations. Figure 2 shows the dependence of the temperature of the surface layer on time during processing in the adiabatic mode with melting of the steel surface - the right side of equation (7) is equal to zero. When heated (1) to the solidus temperature, the rate of increase in the temperature of the metal decreases. The energy of the heat source is spent on the phase transition. Next, the liquid metal is heated \((T > T_{\text{linc}})\). During cooling due to heat removal into the sample, the opposite process occurs. At the cooling temperature, a relatively smooth temperature drop occurs, associated with the solidification of the liquid phase. Similar to the one described above, the less obvious pronounced character of the temperature behavior at \(\alpha \rightarrow \gamma\) and \(\gamma \rightarrow \alpha\) transitions.

Samples made of U8 steel were treated with an electron beam ejected into the atmosphere, the energy in the beam was \(E = 1.5\) MeV, and the processing time was \(\tau = 1\) ms. Figures 2 and 3 show the structures of the heat-affected zone obtained after treatment with an electron beam in the adiabatic mode with reflow (specific energy release \(Q = 6.2\) MJ/m\(^2\)) and without reflow, respectively (specific energy release \(Q = 5.6\) MJ/m\(^2\)). It is seen that the compared calculation does not contradict the experiment.

Figures 4 and 5 show the calculations of the temperature-time dependence for the processing mode with partial reflow and without reflow.

**Figure 2.** The structure of the steel in the thermal heating zone after treatment with partial surface melting.

**Figure 3.** The structure of the steel in the thermal heating zone after processing without reflow.
The compared experimental and calculated data agree within the error limits. The non-uniformity of the cooling curve is related to the phase transition energy, i.e. energy is released from the steel, and slows down the temperature drop. Figure 6 shows the temperature distribution at increased processing power, which leads to excessive heating, followed by melting of the surface. The calculation was carried out in the same way as for Figure 4, only the dependences $T(z)$ are given at different times from the beginning of heating.

The dependencies in Figure 5 are plotted at three characteristic depths, but they reflect the calculation at the most optimal processing mode without reflow: $Q = 5.6 \text{ MJ/m}^2$, $\tau = 1.0 \text{ ms}$.

In the two-phase region, during melting and crystallization, the rate of temperature change decreases. The subsurface nature of melting is seen at the beginning of the heat release region (up to $1/3$ of the effective path of electrons). Then, the exit of the melting zone to the surface is possible.

On the sample processed under the adiabatic mode with reflow (Figure 2), it can be seen that the depth of the heat-affected zone is 0.66 mm and the boundary is pronounced. At a depth of 0.32–0.66 mm, a solid-state quenching structure is formed. At a depth of 0–0.32 mm, there is a quenching zone from the two-phase region. Structure of hardened martensite zones. Contact with the two-phase region causes melting, which leads to a change in flatness (bumps).

The structure in Figure 3 is obtained in a non-adiabatic mode, the formed structure is martensite.
But the difference between the calculated and experimental data in many practically important places is measured by very small values, for example, at the boundary of the areas of thermal action, the error does not exceed 10–15 µm, which generally corresponds to the permissible errors of experiment and calculation.

The photographs of the treated surface layer of U8 steel shown in Figures 2 and 3 illustrate the adequacy of the mathematical model, which is displayed in the form of applied calculated data on the previously obtained images. But there is a noticeable disagreement between the experimental results and the calculations. There are several reasons for this:

1. The error in setting the processing mode.
2. The error in calculating the model.

In general, it can be argued that the created model adequately describes the distribution of thermal fields in the surface layer. To calculate the thermal fields in other materials, it is necessary to replace the arrays of the thermophysical characteristics of the material being processed. In this case, the model can be considered as universal for describing the thermal fields of the material during pulsed heating.

Considering the type of the mathematical model, it can also be used to calculate the thermal fields arising from the processing of material by other sources of thermal energy: laser, electrical and plasma heat sources, in particular.

It is important to note that the results obtained are not limited to specific values of the characteristics of the electron beam - current, diameter, voltage of the accelerating tube, and processing time. Thus, there is a high degree of freedom in the choice of parameters to achieve the desired result.

4. Conclusion

The created error model is adequate for the quantitative-temporal distribution of temperature fields during pulsed heating of the surface layers of metals and alloys. Also, given the type of mathematical model, it can be applied to other energy sources.

5. References

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