Simulation of structure formation of austenitic steel weld

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Abstract. An integrated model of phase transformations is proposed, which unites the model of changes in the temperature fields of the workpiece during welding and subsequent cooling, as well as a simulation model of phase transformations that occur during cooling of the steel. The developed method allows predicting the amount of residual δ-ferrite in the structure of the weld of austenitic stainless steel, which is necessary to justify the welding conditions.

1. Introduction

Almost all areas of modern production used pipes made of stainless steels and high-temperature alloys, which can be generally divided into seamless and welded. The cost of welded pipes is significantly lower than seamless, but there are a number of limitations of the scope of welded pipes. This is primarily due to the limited wall thickness of the finished product and the structural and phase heterogeneity of the material in the weld zone. Currently, these limitations can be significantly reduced by developing and implementing new welding technologies. The development of such technologies should be based on the results of systemic and applied research. As part of this study, the task was to predict the structure of the weld zone of stainless steel after the application of laser welding. To solve this problem, an integrated model of phase transformations was developed, combining a model of changes in the temperature fields of the workpiece during welding and subsequent cooling, as well as a simulation model of phase transformations occurring during steel cooling.

2. Results

2.1. Thermal field modelling

Taking into account the fact that the pipe thickness can take on different values, two types of models were built:

- Two-dimensional model (based on simplifying assumptions about the constancy of the temperature across the thickness of the pipe at any given time) - for a “thin” pipe;
- Three-dimensional model (taking into account changes in temperature values over the thickness of the pipe) - for a “thick” pipe.

The choice of the first or second of these models for carrying out work calculations must be justified by the specific thickness value and the characteristics of the pipe material. Taking into account the...
cylindrical shape of the product in question, a cylindrical coordinate system \((r, \varphi, z)\) was used to build both models. In the case of a two-dimensional model, the distribution of heat across the pipe thickness is not simulated, and two coordinates \((\varphi, z)\) are defined to describe the temperature change. The simulation was carried out on the basis of the heat conduction equation \([1, 2]\), written in cylindrical coordinates at a constant value of \(r\) equal to half the diameter of the pipe, taking into account the transfer of heat by convection from both sides of the pipe surface:

\[
\rho \cdot c \cdot \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( \lambda(\varphi, T) \frac{\partial T}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \lambda(\varphi, T) \frac{\partial T}{\partial \varphi} \right) + \frac{2\kappa(T^0 - T)}{h} + q(t, \varphi, z),
\]

(1)

where \(T\) - the temperature
\(t\) - the time (from the start of processing),
\(q\) - the specific power of the heat source (laser),
\(h\) - the wall thickness of the pipe,
\(T_0\) - the temperature of the medium (initial temperature of the pipe),
\(c\) - the specific heat of the material,
\(\lambda = \lambda(\varphi, z, T)\) - the thermal conductivity of the material,
\(\kappa\) - heat transfer coefficient.

The initial condition was set as \(T(0) = T_0\); boundary conditions on the \(z\) coordinate (boundary conditions of the third kind) - in the form:

\[
z = 0: \quad -\lambda \frac{\partial T}{\partial z} = \kappa(T^0 - T), \quad t > 0,
\]

(2)

\[
z = L: \quad \lambda \frac{\partial T}{\partial z} = \kappa(T^0 - T), \quad t > 0.
\]

In addition, according to the coordinate \(\varphi\), the conjugation conditions were specified \([1]\):

\[
T(0+0) = T(2\pi-0), \quad \lambda \frac{\partial T}{\partial \varphi} \bigg|_{\varphi=0} = \lambda \frac{\partial T}{\partial \varphi} \bigg|_{\varphi=2\pi-0}.
\]

(3)

The solution of equation (1) was performed by the finite difference method. For this purpose, uniform spatial and temporal grids were introduced.

Replacement of partial derivatives with respect to coordinates by difference analogues was carried out according to an explicitly implicit scheme (an explicit scheme for \(\lambda\), implicit in \(T\)) according to the method described in \([1]\). Difference equations approximating equation (1), boundary conditions (2), and conjugation conditions (3) have the form:

\[
\frac{1}{r^2} \frac{\lambda^v_{i+1,j}^{l+1} + \lambda^x_{i,j}^{l+1}}{h^v_{i+1} + \lambda^x_{i,j}^{l+1}} \cdot T_{v,i+1,j}^{n+1} + \left( \frac{\rho \cdot c}{\tau} + \frac{\lambda^x_{i,j}^{l+1}}{r^2 \cdot h^v_{i+1} + \lambda^x_{i,j}^{l+1}} \right) \cdot T_{v,i,j}^{n+1} = \frac{2\kappa}{h} \cdot \frac{T^0 - T_{v,i,j}^{n}}{\tau} + q_v^n,
\]

(4)

\[
T_{0,i+1,j}^{n+1} = \frac{\lambda^x_{i+1,j}^{l+1} + \kappa \cdot h_i \cdot T^0}{\lambda^x_{i+1,j}^{l+1} + \kappa \cdot h_i}, \quad T_{v,i,j}^{n+1} = \frac{\lambda^x_{i,j}^{l+1} \cdot T_{v,i,j}^{n+1} + \kappa \cdot h_i \cdot T^0}{\lambda^x_{i,j}^{l+1} + \kappa \cdot h_i},
\]

(5)

\[
T_{ij} = T_{v,i,j}^{n}, \quad T_{2j} = T_{v,2,j}^{n}, \quad T_{ij} = T_{v,i,j}^{n+1}.
\]

(6)
\[ T^0_{ij} = T^0, \quad i = 2, 3, \ldots, N_\varphi - 1, \quad j = 2, 3, \ldots, N_z - 1, \quad n = 0, 1, 2, \ldots, \]

where \( h_0 \) - the step value by \( q \),
\( h_x \) - the value of the step in \( z \),
\[ \lambda_{ij}^n = \frac{\lambda_{ij} + \lambda_{i+1,j}}{2}, \quad \lambda_{i,j}^n = \frac{\lambda_{i,j} + \lambda_{i,j+1}^n}{2}, \]
\[ \lambda_{i,j}^n = \frac{\lambda_{i,j}^n + \lambda_{i-1,j}}{2}, \quad \lambda_{i,j}^n = \lambda(T^0_{ij}), \]
\[ q_{ij}^n = \begin{cases} q, & \text{where } \varphi = \left\lfloor \frac{N_\varphi}{2} \right\rfloor + 1, \quad j = n + 1, \quad n = 0, 1, \ldots, N_z - 1, \\ 0, & \text{otherwise}. \end{cases} \]

\( q \) - the radiation power density at the welding point,
\( \lfloor \cdot \rfloor \) - the integer part of number.

The requirement \( j = n + 1 \) is due to the choice of the time step (it is assumed that the laser shifts one step along the \( z \) axis in one time step); the condition \( n \leq N_z - 1 \) - termination of laser operation after reaching the end node along the \( z \) coordinate.

To obtain the temperature field at the \( n \)th time step, it is necessary to determine the values from the obtained relations for \( T^0_{ij} \). At step \( n = 0 \), the initial conditions are also used.

Using relations (4) - (6), it is possible to determine both the heating modes of the welding zone and the modes of its subsequent cooling. To carry out the corresponding calculations, software was developed that allows determining the temperature values for all points of the simulated region at a given point in time.

2.2. Simulation of phase transformations

Most mathematical models of the kinetics of phase transformations are constructed for isothermal conditions based on the Kolmogorov crystallization equation or the Avrami equation. Using these equations to model the transformation with continuous cooling allows us to obtain only qualitative agreement with the experimental data, therefore, in this study, we used a different approach based on the simulation process modeling. In [3, 4], simulation models of the decomposition of supercooled austenite are described, taking into account both the homogeneous and heterogeneous character of the nucleation of a new phase. These models, like the Kolmogorov model, are based on the idea of the nucleation of the centers of the new phase in the volume, initially occupied by the old phase, and the nucleation occurs not simultaneously, but is distributed in time. The use of this approach allowed us to develop a simulation model for predicting the kinetics of austenite decomposition during the heat treatment of powder structural steels, as well as the software package implementing this model. On the one hand, the successful application of simulation methods [3, 4] gives grounds to formulate a hypothesis about the applicability of this methodology to the description of the kinetics of phase transformations for materials of different chemical composition. On the other hand, an analysis of the processes occurring during the cooling of austenitic stainless steels from the melting point to room temperature shows a slightly different picture of the transformations.

According to [5, 6], when studying the transformation of \( \delta \)-ferrite in the process of cooling austenitic stainless steel, several temperature ranges should be distinguished. In the first (upper) temperature range, \( \delta \)-ferrite, formed during crystallization, interacts with the liquid metal, as a result of which austenite is formed by the peritectic reaction. When the temperature drops below the solidus temperature, \( \delta \)-ferrite dissolves in austenite (transformation in the solid phase). The authors note that with a further decrease in temperature as a result of the eutectoid reaction, the release of ferrite from austenite may begin, but the development of this process is kinetically inhibited and may not be taken into account. Thus, having data on the volume fraction of \( \delta \)-ferrite in the alloy at the time of the end of crystallization, one can
concentrate only on modeling the dissolution of ferrite in austenite in the solid state. In this case, in the case of using simulation modeling, it is necessary to make significant changes to the imitating algorithms described in [3, 4]. The main change consists in the following: instead of imitating the process of nucleation and growth of grains of a new phase in the volume initially occupied by the old phase, it is necessary to realize the reduction (up to disappearance) of the grains of one of the two phases that initially exist in the existing volume of the alloy.

The simulation model developed in the framework of this study is based on the following scheme.

- In space, a certain region is set (simulated volume), which at the initial moment of time is occupied by grains of two phases (δ-ferrite and austenite).
- The simulated volume is divided into fragments (grains). The grain boundaries are given by the equations of the planes, each of which is assigned a number.
- A certain number of fragments (in accordance with the initial fraction of δ-ferrite) is marked as δ-ferrite grains; the remaining fragments are like austenite grains.
- In the process of cooling the simulated volume, the δ-ferrite grain boundaries shift towards decreasing the volume of these grains, up to their complete disappearance.
- The rate of displacement of the boundaries (i.e., the dissolution rate of ferrite grains) decreases with decreasing temperature. In addition, it is assumed that while maintaining a constant temperature, the speed of movement of the boundaries slows down with time due to a decrease in the difference in concentrations.

To build a simulating algorithm, the principle “from event to event” was used. The next event is the beginning of the process of dissolving some grain of δ-ferrite. In addition, each event is characterized by the onset time τ_j and the number of δ-ferrite grain involved in the process of phase transformation. When constructing a model, it was assumed that the flow τ_j of the moments of occurrence of events and the flow of the corresponding grain numbers can be described separately as independent random objects by the corresponding distribution laws. The sequence of moments of the occurrence of events was seen as a uniform flow. Based on the physical laws of the phase transformation process, it was assumed that this flow is the simplest (stationary Poisson) flow, and, therefore, the time between the occurrences of two “neighboring” events has an exponential distribution with the parameter λ, where λ is the flow intensity. If the flow intensity is set, then the moments τ_1, τ_2, ..., τ_k, ... of the appearance of the centers of the new phase can be expressed by the relations:

\[ \tau_1 = t_1, \quad \tau_2 = t_1 + t_2, \quad \ldots, \quad \tau_k = t_1 + t_2 + \ldots + t_k, \quad \ldots \]

where t_1 is the time of occurrence of the first event, t_k, k = 2, 3, ... is the time between the occurrences of the (k-1)-th and k-th event, is a sequence of pseudo-random numbers with exponential distribution with the parameter λ. The number of δ-ferrite grains, for which the phase transformation process was initiated, was determined by generating a uniformly distributed pseudo-random number.

The dependence of the speed of movement of the boundaries on temperature was described by \( e^{\frac{1}{T}} \), the expression where l_1 is the parameter to be determined. In addition, the slowdown factor was taken into account with the time elapsed from the beginning of the transformation \( e^{-\frac{t_1}{l}} \), and, thus, the speed of movement of the boundaries was described by the expression \( l = e^{\frac{1}{T}} \cdot e^{-\frac{t_1}{l}} \). During the operation of the simulating algorithm, at each instant of the next event, the volume fraction occupied by undissolved δ-ferrite \( V_T(\lambda, l_1, l_2) \). The Monte Carlo method was used to determine this volume.

The kinetics of the process of formation of a new phase in this model is determined by the following parameters:

- \( v_0 \) is the volume fraction of δ-ferrite at the initial moment of time,
- \( \lambda \) is the intensity of the flow of events (the beginning of the decay of the δ-ferrite grains),
• \( l_1 \) and \( l_2 \) are the parameters determining the linear velocity of movement of the grain boundaries of the \( \delta \)-ferrite.

The parameter \( v_0 \) depends on the heating conditions and the subsequent cooling of the material, due to the speed of the laser; the parameters \( \lambda, l_1 \) and \( l_2 \) depend on the temperature at which the \( \delta \)-ferrite is dissolved.

Software was developed to allow a computer experiment, during which, according to the scheme described above, for a given set of values of kinetic parameters corresponding to temperature \( T \), the actual process of phase transformation was simulated, and the fraction of undissolved \( \delta \)-ferrite was calculated \( V_T(\lambda, l_1, l_2, t) \) depending on time \( t \). The modeling process continued until the \( \delta \)-ferrite was completely dissolved or until the time point corresponding to the end of the real experiment. The procedure for determining the optimal values of the model parameters was worked out on the available experimental data on the kinetics of dissolution of \( \delta \)-ferrite in austenitic stainless steel with 17.3% Cr and 9.4% Ni [6]. To obtain the values of the kinetic parameters, the sum of squared deviations of the function \( V_T(\lambda, l_1, l_2, t) \) from the experimental values was minimized. The Nelder-Mead method was used as an optimization method [7]. In order to reduce the influence of random factors (distribution of \( \delta \)-ferrite grains in the initial volume and moments of onset of dissolution of individual grains) on the result of a simulation experiment, for each set of parameters, 10 model runs were performed, the results of which were used to plot the average phase transformation curve.

The dependence of temperature on time was modeled on the basis of the heat equation, as described above. The dependence of the kinetic parameters of the transformation on temperature was described by linear interpolation of the values of the model parameters obtained as a result of optimization at the stage of modeling the transformation under isothermal conditions. Modeling of phase transformations with continuous cooling, as in the case of isothermal transformations, was carried out according to the principle “from event to event”. On the basis of the current values of the kinetic parameters, the moment of time corresponding to the onset of the next event was determined. At this time, the temperature value was determined, and the values of the model parameters corresponding to this temperature were calculated; the volume of undissolved \( \delta \)-ferrite was determined. New parameter values become current. The modeling process continued until reaching room temperature.

2.3. Simulation results obtained

The process of heating the weld zone with a focused laser beam, as well as its subsequent cooling, was simulated for various values of radiation power ranging from 1 to 6 kW and values of the laser beam speed from 0.12 m/min to 3.0 m/min. The calculations were performed for a pipe with a diameter of 10 cm and a thickness of 2 to 10 mm. It was assumed that at the indicated pipe wall thickness the process of heat distribution would be adequately described by model (4) - (6). The value of the radiation power density \( q \) at the welding point was determined taking into account the distance between the nodes and the speed of the laser. The calculations were performed for austenitic stainless steel 12X18H10T of standard chemical composition: 17-19% Cr, 9-11% Ni and 0.8% Ti.

For each of the simulated welding modes, temperature fields were calculated (temperature values for all nodes of the spatial grid) depending on time. The maximum temperatures reached in the weld zone and the heat-affected zone, as well as the cooling rate at various distances from the laser line of motion, were analyzed. In figure 1 shows the results of calculations for a pipe 2 mm thick with a radiation power of 1 kW and a laser speed of 0.5 m / min: temperature vs. time at a point on the laser line of motion.
After calculating the temperature fields and, as a result, determining the cooling modes of the heat-affected zone, the δ-ferrite dissolution process was simulated, which occurs with a decrease in temperature after welding is completed. For each value of the pipe thickness, only those welding conditions were analyzed that ensured the achievement of a temperature sufficient to melt the material. The determination of the volume fraction of residual δ-ferrite and austenite in the steel structure was performed in accordance with the algorithms described above. The amount of residual δ-ferrite was mainly analyzed. Table 1 presents the results obtained for several modes of welding of a pipe 2 mm thick. As calculations show, the share of residual ferrite in the weld zone does not exceed 5% for all the considered modes.

Table 1. The amount of residual δ-ferrite in the weld zone under different welding conditions. Pipe thickness 2 mm.

| Welding mode (power, laser speed) | The share of residual δ-ferrite, % |
|----------------------------------|-----------------------------------|
| Q = 1 kW; v = 0.5 m/min          | 5                                 |
| Q = 2 kW; v = 1 m/min            | 1.8                               |
| Q = 3 kW; v = 2 m/min            | 1.4                               |
| Q = 5 kW; v = 3 m/min            | 0.55                              |

3. Conclusion
An integrated model of phase transformations in the weld zone has been developed, including a model of the temperature fields of the workpiece and a simulation model of phase transformations occurring during cooling of the steel; developed software that implements this model. The proposed method allows us to predict the amount of residual δ-ferrite in the weld structure of austenitic stainless steel after cooling the pipe. This technique can be useful for justifying the modes of laser welding of pipes made of austenitic stainless steels in terms of achieving the required quality indicators of the finished product.

It is shown that the method of simulation of phase transformations used to predict the structure of structural steels after heat treatment [3, 4] after modification can be used to simulate the structure formation in the weld zone of austenitic steel.

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References
[1] Samarsky A A 1977 Difference Scheme Theory (Moscow: Nauka)
[2] Samarsky A A, Tikhonov A N 1977 Equations of Mathematical Physics (Moscow: Nauka)
[3] Ivashko A G, Tsyganova M S and Nabatov R I 2016 Decomposition kinetics of supercooled austenite in porous powder steel Steel in Translation (vol. 46) No. 3, pp. 196–200
[4] Tsyganova M S, Ivashko A G, Polyshuk I N, Nabatov R I and Tsyganova A I 2017 Simulation of
decomposition kinetics of supercooled austenite in powder steel *IOP Conf. Series: Earth and Environmental Science (Electronic Materials* vol. 87)

[5] Kazakov A A, Oryshchenko A S, Fomina O V, Zhitenev A I and Vikhareva T V 2017 Control of delta-ferrite nature in nitrogen-containing chromium-nickelmanganese steels *Voprosy Materialovedeniya* (No 1 (89)) pp. 7–21

[6] Saied M 2016 *Experimental and Numerical Modeling of The Dissolution of Delta Ferrite In The Fe-Cr-Ni System: Application to the Austenitic Stainless Steels Materials* (Grenoble: Université Grenoble Alpes)

[7] Bunday B D 1984 *Basic Optimization Methods* (London: Edward Arnold)