COMPUTER SYSTEM FOR PREDICTING THE STRUCTURE AND PROPERTIES OF CAST METAL PRODUCTS

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Abstract: The basic principles of functioning of subsystems of the information-technological complex, which is intended for the forecast of structure and properties of the cast metal, are presented. The basis of subsystems are mathematical and simulation models of crystallization. The subsystem of thermal analysis is based on mathematical models, which were developed within the framework of the dynamic theory of metallic castings The subsystem of modeling of crystallization is based on a combination of mathematical models of heat conduction and diffusion with cellular automata. The model makes it possible to investigate in computational experiment the effect of various cooling conditions on the process of formation of the structure during crystallization. The results of computer experiment are shown.

KEYWORDS: *COMPUTER THERMAL ANALYSIS, SIMULATION MODELING, CRYSTALLIZATION, STRUCTURE OF METALS AND ALLOYS, COMPUTER MODELING, CELLULAR AUTOMATON*

1. Introduction

One of the factors to solve the problem of improving the quality of castings and increasing the efficiency of foundry production is the availability of methods for the on-line monitoring of the melting process and evaluation of the melt's state immediately before casting. Although the process of forming the quality of metal products is complex and multistage, crystallization plays a special role in it since it is at this stage the "primary" structure of solid metal is formed, which significantly influences the formation of the properties, which the final product must have. That is, it is necessary to be able to on-line check of the melt's state and control the crystallization process during the technological process of smelting. As one of the variants of realization of this task it is possible to use information-technological complex consisting of subsystems of computer thermal analysis [1] and of simulation modeling of metals' and alloys' crystallization [2]. Thermal analysis provides information on thermal effects during hardening of sample, which reflect the processes of formation of the cast metal's structure. This makes it possible to analyze the kinetics of the crystallization process using data of the cooling curve and to predict the service properties of metals and alloys in the solid state. Simulation modeling makes it possible in the mode of computer experiment to optimize known and develop new technological modes for creating foundry products, which significantly reduces time of development and material costs, gives an opportunity to obtain important scientific information about the process of crystallization of metals and alloys under both equilibrium and nonequilibrium conditions (even those ones, which is difficult or impossible to obtain under in laboratory conditions). Simulation modeling makes it possible in the mode of computer experiment to optimize known and develop new technological modes for creating foundry products, which significantly reduces time of development and material costs, gives an opportunity to obtain important scientific information about the process of crystallization of metals and alloys under both equilibrium and nonequilibrium conditions.

2. Preconditions and means for resolving the problem

The thermal analysis subsystem should record the change of the temperature of metallic material, which is in the process of crystallization (the cooling curve). Using the data of the cooling curve with the help of mathematical modeling it is possible to single out information on the dynamics of the crystallization process, which helps to predict the properties of metals or alloys in the solid state. Mathematical models in this case should be simple, since the calculations based on them must be performed in the computer for the minimum possible time [3]. Similar models are proposed in the framework of the dynamic theory of hardening of metallic castings [4]. Based on these models, a technique for computer thermal analysis is proposed, which simulates differential thermal analysis using the hardware of simple thermal analysis. The application of this technique significantly increases the sensitivity of the method, as well as the reliability of the forecast of the structure and properties of the metal in the solid state.

In the process of developing of a subsystem of simulation modeling of the formation of the structure of metallic materials during their crystallization, problems arise due to the complexity of the mathematical formulation of the problem. At the same time, studies of cellular automata have shown the principal possibility of their use for modeling of similar processes [5]. However, the rules for cellular automata' operation of are usually given without connection with real physical processes. In this paper we propose a simulation model of crystallization, which is based on combination of mathematical models of heat conduction and diffusion with cellular automata. At that, the external cooling conditions and composition of the liquid metal or melt at a certain point determine the possible state (liquid or solid) of the corresponding cell of the cellular automaton.

3. Structure and capabilities of the models

3.1. The subsystem of computer thermal analysis

Mathematical difficulties which arise while creating mathematical models of crystallization can be significantly reduced if we consider the case of solidification of a body whose temperature gradient across its volume can be neglected. In the method of thermal analysis, which is used in this work, portions of metal or metal alloys which have small dimensions and cylindrical shape with a diameter of 20 ... 40 mm are examined. Since metallic materials are good conductors of heat, in this case it is possible to proceed to an analysis of the heat balance equation for the whole sample as a whole [4]. Then the heat balance equation is represented as:

$$\frac{dQ}{dt}=\frac{dQ_c}{dt}+\frac{dQ_L}{dt}, \tag{1}$$

where $\frac{dQ}{dt}$ - the change in the amount of heat in the sample due to its release into the environment; $\frac{dQ_L}{dt}$ - change in the amount of heat, which is released as a result of formation of a solid phase; $\frac{dQ_c}{dt}$ - change in the amount of heat in the sample due to changes of the material's temperature.

Substituting the known relations in (1):

$$dQ_c=-cmd(t), \tag{2}$$

$$\frac{dQ}{dt}=fS\left[T(t)-T_{cp}\right]+\sigma\varepsilon S\left[T^4(t)-T_{cp}{}^4\right], \tag{3}$$

we obtain the differential equation in the form:

$$\frac{dT(t)}{dt}+k_1\left[T(t)-T_{cp}\right]+k_2\left[T^4(t)-T^4{}_{cp}\right]=Z(t), \tag{4}$$

where $$Z(t)=\begin{cases}0, & \text{при } t\le t_{кр},\ t\ge t_{тв}\\ \frac{L}{c}\frac{m(t)}{m_0}, & \text{при } t_{кр}\le t\le t_{тв}\end{cases} \tag{5}$$

$$V(t)=\frac{m(t)}{m_0}, \quad (6)$$

$$k_1=\frac{fS}{cm_0}, \quad (7)$$

$$k_2=\frac{\sigma\varepsilon S}{cm_0}, \quad (8)$$

where $T(t)$, T_{cp} - are the temperatures of the metal (of cooling curve) and of the environment; t - is the total time of the process; $t_{кр}$ - is the time of onset of crystallization; $t_{тв}$ - time of the end of crystallization; c, L, m_0 – are, respectively, specific heat, specific latent heat of crystallization and portion's mass of the material that is being investigated; $m(t)$ - is the mass of the solidified part of the sample to the instant t; ε - is the degree of blackness of the cooling surface; $\sigma = 5{,}56\cdot10^{-8}$ Дж/(м·К^4) – is the Stefan-Boltzmann constant.

Equation (4) simulates the technique of differential thermal analysis, which has a high sensitivity of the beginning and end of phase transformations. During the experiment, the cooling curve $T(t)$ is fixed in the computer memory. Then, its fourth degree and derivative are calculated. Knowing the values of the coefficients k1, k2, we can calculate the right-hand side of Z (t) equation (3). Before the beginning of crystallization and after its termination, the value of Z is zero. During crystallization, heat is released and the balance is disrupted. These changes at the points $t_{кр}$ and $t_{тв}$ are easily recorded in the experiment.

To determine the values of the coefficients k_1 and k_2, the initial and final sections of the cooling curve are used, where there is no release of crystallization heat and the right-hand side of equation (4) is zero. These sections of the cooling curve are linearized by dividing of both parts (4) by $[T(t)-T_{cp}]$ and introducing of new variables:

$$x=\frac{T^4(t)-T_{cp}^4}{T(t)-T_{cp}}, \quad (9)$$

$$y=-\frac{T'(t)}{T(t)-T_{cp}}. \quad (10)$$

Then equation (4) in these areas becomes the equation of a straight line:

$$y=k_1+k_2x. \quad (11)$$

The values of the coefficients are determined by the method of least squares [6].

Thus, this technique of computer thermal analysis uses the hardware part of simple thermal analysis and simulates differential thermal analysis. Its use in the subsystem of the computer thermal analysis makes it possible to analyze the kinetics of the crystallization process using the data of the cooling curve and to predict the service properties of metals in the solid state.

3.2. The subsystem of simulation modeling

The two-dimensional heat equation is used in the development of the subsystem of simulation modeling of formation of the structure of metallic materials during their crystallization. It assumes that cooling of the body comes from all four sides of the plane, and thermophysical characteristics of the melt (specific heat, density and thermal conductivity) do not depend on temperature (ie, c, ρ, λ = const):

$$\frac{\partial T(x,y,t)}{\partial t}=a\left(\frac{\partial^2T(x,y,t)}{\partial x^2}+\frac{\partial^2T(x,y,t)}{\partial y^2}\right)\pm\frac{L}{c}\frac{\partial\varepsilon(x,y,t)}{\partial t}, \quad (12)$$

$$T(x,y,0)=T_0=const, \quad (13)$$

$$\frac{\partial T(0,y,t)}{\partial x}=-\alpha_1[T(0,y,t)-T_0], \quad (14)$$

$$\frac{\partial T(x_0,y,t)}{\partial x}=-\alpha_2[T(x_0,y,t)-T_0], \quad (15)$$

$$\frac{\partial T(x,0,t)}{\partial y}=-\alpha_3[T(x,0,t)-T_0], \quad (16)$$

$$\frac{\partial T(x,y_0,t)}{\partial y}=-\alpha_4[T(x,y_0,t)-T_0], \quad (17)$$

where $a=\frac{\lambda}{c\rho}$ - is the coefficient of thermal diffusivity; $\varepsilon(x, y, t)$ - is the fraction of the solid phase in some elementary volume; T_0 - is the initial temperature; L - is the specific latent heat of crystallization; α_1, α_2, α_3, α_4 - heat transfer coefficients from four sides; x_0, y_0 - are the dimensions of the system. The last term in the heat equation.

The last term in the heat equation (12) takes into account the release (or absorption) of heat during the phase transformation. Since a cellular automaton is used in the simulation model of crystallization, it is convenient to solve this problem numerically. This solution is realized by the splitting method using an implicit numerical scheme.

Taking into account the need to enter the system time in the model, the order of calculations is organized as follows. First and foremost, the heat conduction problem is solved numerically, in which the time step determines the system time of the entire model. At that, one step of the system time is the total time of observation of the diffusion problem. Therefore, the calculation of this task is carried out anew at each step of the system time. At that, the initial condition changes each time: the previous solution becomes a new initial condition. The boundary conditions assume the absence of exchange of matters at the boundaries of the system:

$$\frac{\partial K(x,y,t)}{\partial t}=D\left(\frac{\partial^2K(x,y,t)}{\partial x^2}+\frac{\partial^2K(x,y,t)}{\partial y^2}\right), \quad (18)$$

$$K(x,y,0)=K_0(x,y), \quad (19)$$

$$\frac{\partial K(0,y,t)}{\partial x}=0, \quad (20)$$

$$\frac{\partial K(x_0,y,t)}{\partial x}=0, \quad (21)$$

$$\frac{\partial K(x,0,t)}{\partial y}=0, \quad (22)$$

$$\frac{\partial K(x,y_0,t)}{\partial y}=0, \quad (23)$$

where $K(x,y,t)$ -) is concentration of the second component in the melt; $K_0(x,y,)$ - is an initial concentration, which is updated at each step of the system time; D - is the diffusion coefficient of the second component of the alloy in the melt. The solution of this problem is completely analogous to the solution of the thermal problem.

The temperature and concentration of the second component at each point of melt determine the size of the local supercooling, which is calculated as the difference of the liquidus temperature for this point and its temperature at a given time. Subcooling in the liquid state is the main driving force of crystallization. In its presence, there are conditions for formation of a crystal or growth of an already existing embryo. To calculate the presence and magnitude of supercooling, the linearization of the liquidus lines and of the solidus of the double-alloy state diagram with the eutectic is used.

Thus, in the subsystem of simulation modeling, mathematical models of heat conduction and diffusion are organized in such a way that it is possible to simulate various conditions of cooling which take place during crystallization in the technological processes of foundry. The simulation model itself has the possibility of changing the cooling conditions (reducing or increasing the intensity of the heat removal) directly in the course of the computer experiment.

4. Results and discussion

The basis for predicting of the mechanical properties of the alloys of the AL-Si and Al-Si-Mg systems in the cast state is that the temporary tear resistance $\sigma_в$ and relative elongation δ are mainly determined by the chemical composition of alloys' main alloying components (Si, Mg) and impurities, which significantly affect the mechanical properties of these alloys (for example, Fe). In addition,

inherited metal's properties and technology's factors that are difficult to control (for example, overheating or modifying) can also change the average level of mechanical properties. The total effect of these factors is manifested in the thermogram in the form of a change in the values of recalescence during the formation of the **α**-phase and the eutectic. As shown in [3], these parameters, in particular eutectic recalescence, correlate with the level of mechanical properties. Therefore, it is advisable to introduce its value as an additional parameter into equation of forecasting of mechanical properties. To create appropriate regression equations, experiments were performed in which content of the silicon for Al-Si and Al-Si-Mg alloys varied from 6.1% to 11.3% and of magnesium - in the range from 0.15% to 0.40%. Equations are obtained for the alloy of the Al-Si system, which bind the temporary tear resistance and relative elongation with the calculated content of silicon, iron, and with the value of eutectic recalescence. They have the following form:

$$\sigma_в = 14{,}37145 + 0{,}31076 \cdot Si - 13{,}1125 \cdot Fe - \\ - 9{,}3304 \cdot Fe^2 + 0{,}2431 \cdot \Delta T_{эр}, \quad (24)$$

$$\delta = 4{,}4195 - 0{,}16663 \cdot Si - 1{,}7786 \cdot Fe - \\ - 1{,}06714 \cdot Fe^2 + 0{,}0283 \cdot \Delta T_{эр}, \quad (25)$$

а для сплава системы Al-Si-Mg:

$$\sigma_в = 51{,}01231 + 4{,}13723 \cdot Si + 8{,}05964 \cdot Mg - \\ - 4{,}6346 \cdot Fe + 0{,}01782 \cdot \Delta T_{эр}, \quad (26)$$

$$\delta = -2{,}1175 - 1{,}3332 \cdot Si - 0{,}2143 \cdot Mg - 5{,}60762 \cdot Fe + \\ + 0{,}0171 \cdot \Delta T_{эр}, \quad (27)$$

where $\Delta T_{эр}$ - the value of the recalescence of temperature, determined by the cooling curve in the region of formation of the eutectic. Composition of alloys is also determined by the cooling curve by means of the method, which is described in [3]. Fisher criterion was used to prove the adequacy of the models, and the error in forecasting of the properties was 5 ... 7%. When testing the subsystem of computer thermal analysis under industrial conditions, the equations described above showed the convergence of results and the accuracy of the prediction of properties at the level of standard methods of mechanical testing.

The use of cellular automata greatly simplifies mathematical calculations while usage of the model and gives the principal possibility of modeling of the emerging polycrystalline structure of metallic materials. The influence of the external cooling conditions of the system under study on the functioning of the cellular automaton makes it possible to establish technological methods for

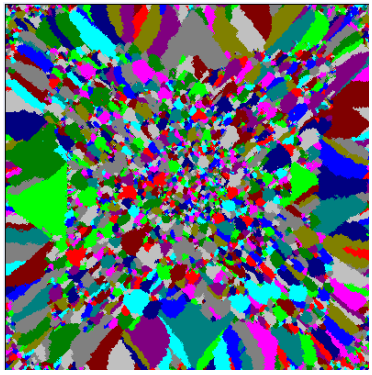

Fig. 1. *Macrostructure of pure aluminum, which is simulated at speed of cooling 5 deg/s*

obtaining various structures of solid metal. Model structures were obtained as a result of the computer experiment of homogeneous crystallization of aluminum with usage of various cooling speed during the process.

With equal speed of heat removal from all sides and a cooling rate of 5 deg/s, a diverse granular structure of pure aluminum is formed (Fig. 1). There are small grains in the center, and on the sides grains' sizes are much larger. It can be also observed that a solid metal's structure is interrelated with the shape of the temperature's field inside the system. Figure 2 shows the structure of aluminum, which

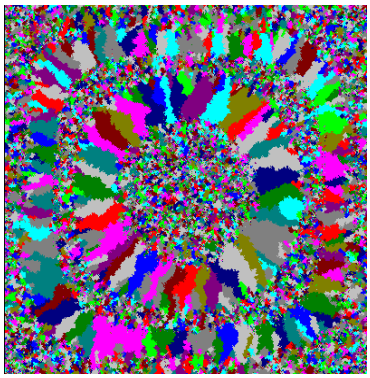

Fig. 2. *Macrostructure of pure aluminum, simulated by an alternate change in the coefficients of heat transfer in the process of crystallization*

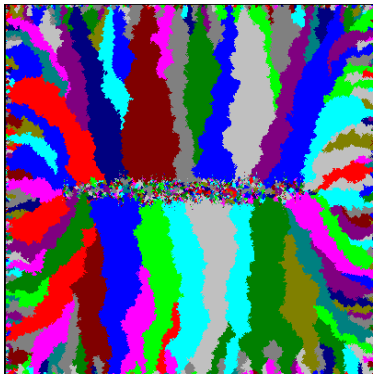

Fig. 3. *Macrostructure of pure aluminum, simulated with asymmetric variation of heat transfer coefficients*

was obtained by repeatedly changing intensity of heat removal. At first, fine grains were formed at the boundaries of the system in conditions of high cooling rate. Then the intensity of heat removal from all sides was reduced symmetrically and the size of the growing grains increased. After some time, the cooling rate was increased, then reduced and then increased again As a result, the final structure consists of several alternating areas with different shapes and different average sizes of grains (Fig. 2). Complex aluminum structure has been obtained in which grains of different shapes, sizes, and orientations are observed (Fig. 3) as a result of varying of the cooling rate by setting asymmetrical coefficients of heat removal from different sides and by varying of their magnitude. It can be assumed that in this case the properties of the real metal will have anisotropy. Such regimes of crystallization are not easy to be realized in practice, but these experiments demonstrate the capabilities of this modeling subsystem.

5. Conclusion

1. Usage of mathematical models of solidification of a small portion of metal allows to increase the sensitivity of thermal analysis to the level of differential thermal analysis due to calculating of the sample's heat balance before, after and during crystallization.
2. The resulting regression equations allow to predict the level of breaking point and relative elongation of alloys of Al-Si and Al-Si-Mg systems using data from the cooling curve of the thermal analysis with an error of 5 ... 7%.
3. Simulation model of crystallization makes it possible to visualize the process of formation of the macro structure of metals under different conditions of crystallization, that makes it possible, within the framework of a computer experiment, to develop techniques for management of this process to obtain the necessary properties of cast products.

4. Combination of the subsystem of simulation modeling of crystallization and subsystem of computer thermal analysis as part of the informational and technological complex significantly expands possibilities of controlling the cast products' quality and allows to obtain information by engineers-technologists both in applied and in theoretical aspects.

6. Literature

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