Simulation of crystallization parameters of casting alloys during modifying treatment by physical impact

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Abstract. The paper presents the developed mathematical model for calculating the crystallization parameters of engineering casting alloys processed by external physical impacts, allowing the critical size of the crystallizing nuclei to be predicted and the amount of nuclei for evaluating the effectiveness of the melt modifying treatment. To automate the calculations for the proposed model, the application software has been created using modern methods of visual software design on the basis of modular and object-oriented approaches. Using A356 aluminum alloy as an example, it was shown that the melt treatment by physical impacts helps to reduce the critical size of the crystallizing nuclei and increase their amount, with the greatest effect being achieved for alloys with a higher proportion of secondary materials in the charge. Prospects of using the calculation technique for the proposed mathematical model in real production conditions during development of technological processes for the production of foundry alloys and castings from them are indicated.

1. Introduction

It is known that the quality of foundry engineering alloys is determined by their structure, which affects the level of mechanical, technological and operational properties of the parts.

At present, methods of physical (external) modifying effects on melts such as ultrasound, vibration, high-temperature superheating, electric current, a magnetic field, etc., are being introduced in the industrial foundry and metallurgical technologies [1-5]. These effects promote the formation of a fine-grained structure and increase the mechanical and operational properties of castings without the introduction of special modifying additives, in some cases having a rather high cost. The main advantage of physical influences is that they do not change the chemical composition of the melt and do not lead to the accumulation of undesirable impurities in casting alloys during further remelting [6-8]. In this regard, the use of physical effects conditions the prospects of using an increased number of secondary materials during melting.
The aim of the work consists in the development and approbation of a computational model for calculating the critical size of the nucleus and the number of nuclei in the melt volume during the modifying treatment of melts using physical methods of action.

2. Methods

The influence of physical effects on the melt is proposed to be interpreted from the position of the cluster model [8]. In accordance with the cluster model of the structure of melts, the main structural components of the liquid are considered separate clusters surrounded by a three-dimensional grid of a disordered zone with a chaotic atomic structure [9]. Clusters in microvolumes can be of different size, composition and density. The internal atomic structure of clusters is close to the structure of the original solid. The characteristic cluster size has a nanoscale that does not exceed the dimensions of the critical nucleus ($r_c$).

Taking into account the modern concepts of the cluster model, the following expressions were obtained by mathematical transformations for spherically formed nuclei:

$$r_c = \frac{3J\Delta W}{e\rho L} \left(\frac{\Delta T}{\Delta \tau}\right)^{-1}, \quad (1)$$

$$n_0 = \frac{3c\Delta T_s}{4\pi L} \frac{1}{r_c^3}, \quad (2)$$

where $J$ – current pulse due to the transition of electrons from the ionization level of the free atom in the disordered zone to the level Fermi nucleus (cluster); $\frac{\Delta W}{e}$ – jump of a potential at the boundary of cluster with a disordered zone; $\Delta W = (J_1 - W_{lib})$ – the work expended by the valence electron upon transition to the level Fermi cluster when a nucleus of critical dimensions is formed; $J_1$ – the first potential of ionization; $W_{lib}$ – the work of the electron liberation; $T_0$ – the equilibrium temperature of crystallization; $\frac{\Delta T}{\Delta \tau}$ – rate of melt cooling in the period of crystals nucleation; $n_0$ – the number of nuclei per unit volume of the melt; $\rho$ – density; $L$ and $c$ – the specific heat of crystallization and the heat capacity of the melt; $\Delta T_s$ – supercooling of the melt.

This mathematical model is universal and allows the main parameters of melts crystallization (the critical size of the nucleus $r_c$ and the number of nuclei per unit volume of the melt $n_0$) to be predicted after their treatment by various physical effects.

For the automation of calculations based on the proposed model, the original software “Calculation of melt crystallization parameters after treatment external actions” was developed using modern methods of visual design of computer software based on modular and object-oriented approaches. Delphi integrated development environment was used to create the calculation modules. The thermophysical properties of the substances incorporated in the program database and open for additions or changes serve as the initial data for the calculations. The program makes it possible to calculate the critical radius of the nuclei $r_c$, the number of nuclei per unit volume of the melt $n_0$, depending on the experimentally determined crystallization parameters – supercooling of the melt and the nucleation time interval. It is possible to simultaneously calculate both $r_c$ and $n_0$ for the initial melt; the melt after physical action (magnetic field, electric current, vibration, inert gas); the melt with a complex processing technology, as well as visualization of the calculation results.

Calculations can be carried out for the following alloys: carbon steels, cast irons, bronzes, aluminum alloys of various compositions. In the case under consideration, the object of the study was alloy A356 (equivalent to the brand EN AB-42100 in accordance with standard EN 1676-2010, the chemical composition according to table 1), which is now widely used in various industries, including for casting parts of metallurgical engineering (instrument parts, pump cases, carburettors operating at...
temperatures up to +200 °C, etc.). The initial data for determining the crystallization parameters are given in table 2.

Table 1. Chemical composition of alloy A356 according to EN AB-42100, wt%.

| Al  | Si   | Mg    | Fe   | Cu   | Mn   | Zn    | Ti   | Other impurities |
|-----|------|-------|------|------|------|-------|------|------------------|
|     | base | 6.5-7.5 | 0.30-0.45 | ≤0.15 | ≤0.03 | ≤0.10 | ≤0.07 | ≤0.18 | ≤0.03 | ≤0.10 |

Table 2. Reference data for calculating the crystallization parameters of A356 alloy using the proposed model.

| Material | The first ionization potential, eV | Current impulse, A/m² | Work function of electron, eV | Density, kg/m³ | Specific heat of crystallization, J/kg | Heat capacity, J/kg K |
|----------|-----------------------------------|-----------------------|-------------------------------|----------------|----------------------------------------|-----------------------|
| A356     | 5.984                             | 8.134                 | 4.23                          | 2500           | 281 000                                | 1085                  |

The necessary values for the calculation of melt supercooling and the time interval of nucleation during the treatment of A356 alloy by physical actions were determined experimentally by thermal cooling curves. The melting of the experimental alloy and its processing were carried out in the induction furnace IF-0.06. Refining of melts before casting was carried out by manganese chloride (0.2% of the melt mass). The physical effects applied were thermal treatment \( T = 970...980 \, ^\circ C, \tau = 7...10 \, \text{min} \) – with 100 % pig materials in the charge, \( T = 1000...1020 \, ^\circ C, \tau = 10...12 \, \text{min} \) – with 50...100 % of pig materials in the charge), a constant magnetic field with a gradient \( \Delta B/\Delta x = 0.886 \, \text{T/m} \) when casting into a mold, a constant electric current during crystallization \( j = 0.92 \times 10^5 \, \text{A/m}^2 \), and their combinations. The secondary materials in the charge in all options contained in their volume: 50 ... 55% of fine scrap and waste alloys, 45 ... 50% of briquetted shavings of the alloy with the same chemical composition.

3. Results and discussion

Of great interest is the study of the parameters \( r_c \) and \( n_0 \) depending on the quality of the charge used and various methods of physical effects on melts. The results showed a significant influence on the crystallization process of such methods of physical actions as the temperature-time treatment (TTT) and the magnetic field.

Table 3 presents the results of calculations for the developed model using a software application for A356 alloy, obtained from different charge.

Table 3. Calculations results of crystallization parameters of A356 alloy using the software application “Calculation of melt crystallization parameters after treatment external actions”.

| Composition of charge | Method of melt treatment | \( r_c \times 10^{-7} \, \text{m} \) | \( n_0 \times 10^{14} \, \text{m}^{-3} \) |
|----------------------|--------------------------|-----------------------------------|-----------------------------------|
| A356 (pig metals)    | Initial (without treatment) | 0.9253                            | 0.1083                            |
|                      | TTT                      | 0.3322                            | 0.3071                            |
|                      | Magnetic field           | 0.4056                            | 0.2453                            |
|                      | TTT + magnetic field     | 0.2098                            | 0.4669                            |
|                      | Electric current         | 0.4815                            | 0.2173                            |
|                      | TTT + electric current   | 0.3071                            | 0.3291                            |
| A356 (50 % of pig metals + 50 % of secondary) | Initial (without treatment) | 0.9706                            | 0.1029                            |
|                      | TTT                      | 0.3689                            | 0.2688                            |
|                      | Magnetic field           | 0.4588                            | 0.2114                            |
It follows from the data in table 3 that the melts treatment by physical actions (both individually and in a complex) leads to a decrease in the critical radius of the nuclei \( r_c \) and an increase in the number of nuclei per unit volume of the melt \( n_0 \). As a result, because of the bulk character of the crystallization, a fine-grained structure is formed in the alloys. It should be noted that physical actions had a greater effect on the alloy from the charge with an increased amount of secondary materials (scrap and waste).

The presented mathematical model realized in the developed program allows the crystallization parameters \( r_c, n_0 \) to be predicted after applying various physical actions and the effectiveness of a particular technology of modifying melt processing in the production of thin-walled castings of various purposes from ferrous and non-ferrous alloys to be evaluated. For calculation the reference data on the thermophysical properties of materials and the experimentally determined crystallization characteristics of melts are required.

A promising direction for development of the above indicated approaches to predicting the parameters of crystallization can be their adaptation to foundry composite materials on a metal basis [10]. Modifying treatment of metal matrix composites reinforced with endogenous phases (TiB_2, TiC, Al_3Ti, Mg_2Si, etc.) is not only advisable from the standpoint of improving the micro- and macrostructure of the matrix, but also for controlling the morphological characteristics of the forming reinforcing particles. Considering the significant potential of using physical methods of melts treatment for modifying composites, the development of reliable calculation models for evaluating the efficiency of such treatment will allow the most rational technological modes for obtaining composite alloys with specified properties to be choosen.

4. Conclusion
A mathematical model is developed for calculating the crystallization parameters of foundry machine-building alloys treated by physical actions, which allows the critical size and the number of crystallization nuclei for evaluating the effectiveness of the melt modifying treatment to be predicted. The proposed methodology for calculating crystallization parameters can be applied in production and research laboratories and centers dealing with the issues of obtaining high-quality castings for machine-building purposes.

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