Calculations of some thermo-physical properties of aluminum alloys using data of thermal analysis

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Abstract. Increasing the accuracy of computer simulation of the crystallization processes of aluminum alloys and the solidification of castings requires reliable data on the thermo-physical properties of the alloys used. The present paper describes a technique for calculating the heat of crystallization and heat capacity of aluminum alloys in the range from the temperature of its pouring into the mold to the average temperature of the solidified skin according to the results of thermal analysis. The proposed technique can be used to determine the values of thermo-physical properties of aluminum alloys in industrial and research laboratories and centers involved in production of high-quality castings.

1. Introduction

Aluminum alloys are one of the most economical and technologically advanced materials used in industrial foundry technologies in the production of lightweight structural parts [1, 2]. The growing requirements for the quality of cast products from aluminum alloys necessitate the development of new and optimization of existing technological processes of melting and casting [3-5].

Computer simulation of the crystallization processes of aluminum alloys and the solidification of castings from them is currently widely used both in scientific research practice and in industrial conditions for solving problems of increasing the productivity and quality of manufactured castings [6-9]. This approach has repeatedly proved its effectiveness, allowing us to predict the influence of different casting and solidification parameters without expensive experimental studies. The accuracy of forecast estimates in the simulation will be largely determined by the accuracy of the experimental determination or theoretical calculation of the thermo-physical properties of aluminum alloys [10, 11].

Currently, the literature provides limited information on the calculated thermo-physical properties of aluminum alloys with different compositions, and even more so on methods for calculating these properties. Among the published works, it should be noted the studies related to the creation of new methods for determining some required thermo-physical and structural properties for the simulation of cast aluminum alloys using their known chemical composition [12], with development of the tools for

calculation of thermo-physical properties using the CALPHAD approach for modeling of multicomponent alloys [13], and a series of works devoted to the direct calculation of the values of various thermo-physical properties of aluminum alloys [14-16].

However, the reproducibility and accuracy of the results of experimental determination or modeling of the thermo-physical properties of aluminum alloys depends on a wide range of determining factors. We propose to divide this set of factors into four main groups:

1) factors associated with the characteristics of the test sample: mass of the sample; the size of the sample, the location of the measuring sensor in the sample, the shape of the sample holder (from thin plates to deep crucibles), the material of the sample holder (glass, ceramics, metals);

2) factors associated with the conditions of the experiment: the heating/cooling rate of the sample, the temperature gradient in the body of the sample;

3) factors associated with the measuring device: digital recording speed of the measured values; sensitivity of measuring devices, filtering/smoothing systems for the measured signal;

4) factors related to the quality of theoretical models for calculating the thermo-physical properties of aluminum alloys: accepted assumptions, selection of constants, boundary conditions, etc.

Many of these factors are not fully understood in the literature. The difficulty lies in the fact that the created computational models are applicable, as a rule, strictly for specific types of samples and/or devices. On the one hand, this is an attempt to stabilize a large number of external factors at the same level and to simplify the calculation models; on the other hand, this is a loss of information about the structural changes of a multicomponent aluminum alloy during phase transitions.

The present paper describes a technique for calculating the heat of crystallization and heat capacity of aluminum alloys in the range from the temperature of its pouring into the mold to the average temperature of the solidified skin according to the results of thermal analysis.

2. Methods

Total solidification time (τ_f) with perfect contact at the crystallization front and at the “casting - mold" interface for casting of any configuration with an effective size R can be calculated by following equation:

$$\tau_f = \frac{Bb}{2 \cdot a}\left(\frac{b}{\lambda_m} + \frac{1}{\lambda_a}\right)R^2 \tag{1}$$

where τ_f – total solidification time of casting,
λ_m – thermal conductivity of the mold,
λ_a – thermal conductivity of the alloy,
a – coefficient depending on casting configuration: for infinite plate a = 1; for infinite cylinder a = 3; for sphere a = 6;
b — dimensionless coefficient, showing how many times the thickness of the heated layer of the mold is greater than the thickness of the solidified skin of the alloy, and

$$b = \frac{L_{cr}\rho_a + c_a\rho_a\left(T_p - \overline{T}_a\right)}{c_m\rho_m\left(\overline{T}_m - T_m^0\right)} \tag{2}$$

B – coefficient, J/(m^{3}K), defined as

$$B = c_m\rho_m\frac{\overline{T}_m - T_m^0}{T_{cr} - T_m^0} \tag{3}$$

where L_{cr} — heat of crystallization of the alloy, J/kg;
ρ_a, ρ_m — density of the alloy and mold, kg/m^3;
c_a, c_m — heat capacity of the alloy and mold, J/(kg·K);
T_p — pouring temperature, K;
T_{cr} — crystallization temperature, K;

T_m^0, $\overline{T}_m$ — the initial temperature of the mold and the average temperature of the heated layer of the mold, K;

$\overline{T}_a$ — the average temperature of the solidified skin of the alloy, K;

λ_m, λ_a — thermal conductivity of the mold and alloy, W/(m·K);

R — effective size of the casting, $R = V_0/F_0$ (where V_0 and F_0 – volume and surface area of the casting), m.

From expressions (1), (2) and (3), we can derive a formula for determining the heat of crystallization of an alloy:

$$L_{cr} = \frac{b \cdot c_m \rho_m \cdot \left(\overline{T}_m - T_m^0\right)}{\rho_a} - c_a \left(T_p - \overline{T}_a\right) \tag{4}$$

The heat of crystallization of the alloy can also be determined by the results of thermal analysis. The initial data are the values of temperature and its first derivative, measured at each moment of time (figure 1, a). According to these data, the temperatures of liquidus and solidus can be determined, as well as the cooling rate, which is calculated by the formula:

$$m = \frac{1}{T(\tau)} \cdot \frac{dT(\tau)}{d\tau} \tag{5}$$

where $T(\tau)$ — current temperature value, K;

τ — current time point, s.

We accept that the cooling rate depends only on the current temperature and does not depend on other thermo-physical parameters. In the case of a phase transformation, the release of crystallization heat leads to a temperature stop and, in some cases, even to an increase in temperature. Thus, considering the thermal balance of the process, we can assume that the change in the cooling rate ($dT(\tau)/d\tau$) in the crystallization interval directly reflects the solidification process and the release of the heat of crystallization $L_{cr}(\tau)$.Based on this, it is possible to calculate the release of this heat in the time interval ($\tau_0 - \tau_1$), where τ_0 and τ_1 — the time of the beginning and end of the phase transformation, respectively. In this interval, the cooling rate can be determined by the formula:

$$m' = -\frac{1}{T(\tau)} \cdot \frac{dT(\tau)}{d\tau} - \frac{1}{T(\tau) c_a} \cdot \frac{dL_{cr}(\tau)}{d\tau} \tag{6}$$

From (5) and (6) it follows

$$L_{cr} = \int_{\tau_0}^{\tau_1} (m - m') T(\tau) \cdot c_a d\tau \tag{7}$$

If there are no phase transformations, then $dT(\tau)/d\tau$ curve is well approximated by the exponential; therefore, to calculate the heat of crystallization in the time interval ($\tau_0 - \tau_1$) the dependence $dT(\tau)/d\tau$ will have the form (figure 1, b):

$$\frac{dT(\tau)}{d\tau} = e^{a_0 \tau + a_1} \tag{8}$$

where a_0 and a_1 — coefficients.

After taking the logarithm of (8) we get

$$\ln\left(\frac{dT(\tau)}{d\tau}\right) = a_0 \tau + a_1 \tag{9}$$

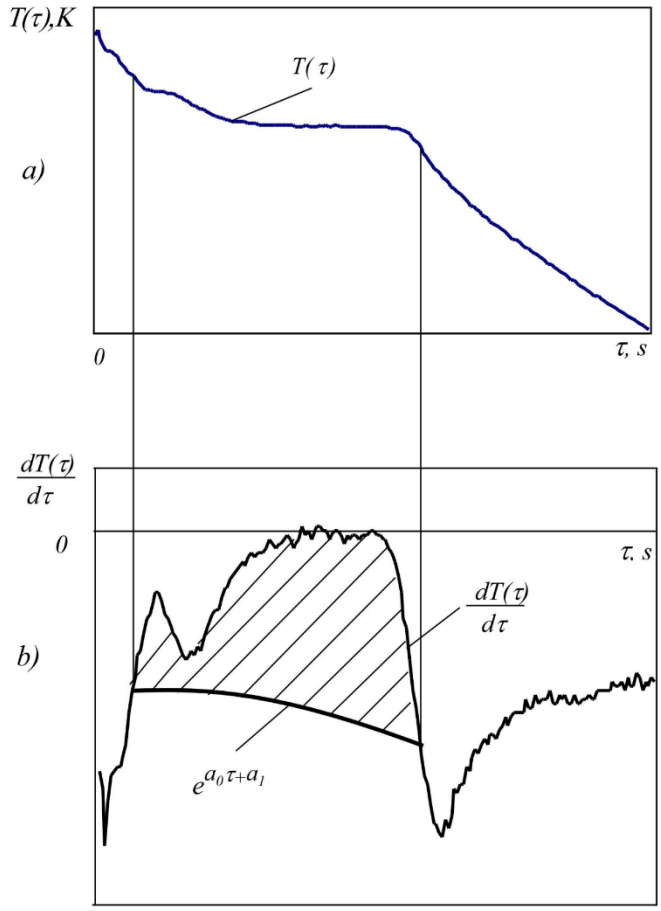

Figure 1. Determination of the heat of crystallization of the alloy according to the results of thermal analysis: a) thermal curve; b) the first derivative of the thermal curve.

To determine the coefficients a_0 and a_1 taking into account the initial conditions, we have a system of equations:

$$\begin{cases} a_0\tau_0 + a_1 = \ln\left(dT(\tau_0)/d\tau_0\right) \\ a_0\tau_1 + a_1 = \ln\left(dT(\tau_1)/d\tau_1\right) \end{cases} \quad (10)$$

Knowing the coefficients a_0 and a_1, we can determine the cooling rate in the time interval ($\tau_0 - \tau_1$) by the formula:

$$m' = -\frac{1}{T(\tau)} \cdot e^{a_0\tau + a_1} \quad (11)$$

3. Results and discussion

By successive transformations from formulas (5), (7) and (11), the computational expression for determining the heat of crystallization of the alloy was obtained:

$$L_{cr} = \int_{\tau_1}^{\tau_0} \left(-\frac{1}{T(\tau)} \cdot \frac{dT(\tau)}{d\tau} - \frac{1}{T(\tau)} \cdot e^{a_0\tau + a_1} \right) T(\tau) c_a d\tau \quad (12)$$

Thus, the heat of crystallization can be determined in two ways: according to formulas (4) and (12). The value of the heat of crystallization, as can be seen from (4) and (12), depends on the thermo-physical parameters: the heat capacity of the alloy and mold, thermal conductivity of the alloy and mold, and density of the alloy and mold, which are functions of temperature and their exact values are often unknown. When calculating heat of crystallization according to one of the methods, ambiguity of solutions may arise: the same value of heat can correspond to different sets of thermo-physical parameters. When using two calculation methods, we can write a system of equations:

$$\begin{cases} L_{cr} = \dfrac{12\tau_f \cdot \left(T_{cr} - T_m^0\right)}{\rho_a \left(\dfrac{1}{\lambda_a} + \dfrac{b}{\lambda_m}\right) R^2} - c_a \left(T_p - 2T_{cr} + \overline{T}_a\right) \\ L_{cr} = \int\limits_{\tau_1}^{\tau_0} \left(-\dfrac{1}{T(\tau)} \cdot \dfrac{dT(\tau)}{d\tau} - \dfrac{1}{T(\tau)} \cdot e^{a_0\tau + a_1} \right) \cdot T(\tau) c_a d\tau \end{cases} \quad (13)$$

The system of equations (13) is determined, and its solution is single-valued under the following assumptions. Since this is a system of two equations, it can be solved with no more than two unknowns. Therefore, in addition to the determined heat of crystallization, it is possible to have one unknown parameter. The heat capacity of the alloy varies over a wide range and has the greatest influence on the calculation results, therefore, factors such as heat capacity, thermal conductivity and density of the mold material, thermal conductivity and density of the alloy are assumed to be constant. Thus, when solving the system of equations (13), the heat of crystallization of the alloy and its average heat capacity can be determined.

Note that the first equation in the system of equations (13) takes into account the average heat capacity of the alloy, i.e., the heat capacity of the alloy in the range from the pouring temperature to the average temperature of the solidified skin of the alloy. This method leads to an underestimation of the average heat capacity of the alloy. Since the system of equations for the heat capacity of the alloy c_a is solved, this fact leads to a decrease in the term $T(\tau)c_a$ and, as a result, to a decrease in the final value of the heat of crystallization. This problem can be solved by dividing the heat capacity of the alloy in the first equation into heat capacity in the liquid state and heat capacity in the solid state. In this case, the heat capacity of the alloy in the liquid state should be substituted into the second equation.

4. Conclusion

A technique for calculating the heat of crystallization and heat capacity of aluminum alloys based on the results of thermal analysis through the solution of an algebraic system of equations with two unknowns is proposed. The technique allows to determine thermo-physical properties according to the results of experimental studies not on standard samples, but directly on a real casting. This is an additional positive side of the proposed technique, because the cooling rate of castings in the mold has a significant effect on the formed structure and the casting defects of a multicomponent aluminum alloy during its transition from a liquid state to a solid state and, as a result, on the estimated thermal properties. An additional measurement and recording of the pouring temperature, the initial temperature of the mold, the average temperature of the heated mold layer and the average temperature of the solidified skin of the alloy can significantly increase the accuracy of the predictive estimates of the thermo-physical properties of aluminum alloys. The calculation algorithm is easily programmed in any algorithmic language or can be implemented using an application package MATLAB for solving technical computing problems.

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