Mathematical simulation of the directional crystallization process

V.I. Bogdanovich, V.P. Golanov, V.G. Smelov, N.V. Nikolaeva
Samara State Aerospace University, 443086, Samara, Russia

Abstract: The paper considers the issues of necessity of use of mathematical simulation of the structuring process by crystallization. Performing such mathematical simulation of the casting process with directed crystallization will allow developing both the theoretical procedure for evaluation of grain of the cast structure and specify the basic requirements to the thermal and physical parameters of the process.

Keywords: Crystallization, dendrite structure, mathematic simulation, liquid-phase, crystallization of the alloy.

INTRODUCTION

The competition at the world market of the aircraft engine building dictates the new requirements for improvement of reliability and efficiency of the gas-turbine engines (GTE) which directly influences the modern ideology of the product quality management during the manufacturing process that in its turn is based on the mathematical simulation of the process within the frameworks of a system approach as well as the establishment of quantitative interrelations between the management and control parameters.

Such approach causes the necessity of the mathematical simulation of the directed crystallization process focused on the maintaining of melting, casting and crystallization of melt in the UVNK-8P units [1]. In these units there has been implemented the principle of directed crystallization by dipping of the ceramic mold with the melt into a liquid-crystal cooler – aluminum cell [1].

During the last decades the steady increase in interest of the national and international researchers in the building of the crystallization models describing the formation of structure of the crystallized melt, chemical inhomogeneity, distributed cast porosity, is observed. These models use the description of processes at different structural levels [2].

In recent decades the issues of mathematical simulation of the crystallization processes are paid an increased attention. To a large extent it is related to the extension of information on the physical properties of alloys, in particular the multi-component molten alloys [3], to the increased complexity of the mathematical models of the physic-chemical crystallization processes [4] and enhanced computing capacity allowing solving the modeling tasks within a short period of time.

Nowadays the mathematic simulation with the use of a computer becomes an efficient tool of researchers and engineers and often is one of the main parts of the computer-aided design systems [5]. Due to the achievements in the modeling area the tasks of forecasting the cast macro-structure by equiaxed and directed crystallization [6], modeling the dendrite crystallization of alloys [7,8] and a number of other topical issues may be solved.

PROCEDURE

The procedure consists in the immediate building of a mathematical simulation model on the basis of which the calculations will be performed.

By mathematic simulation the issues relating to disturbances of the investigated processes by the sensors used during the experiments are eliminated4 there are no technical issues caused by the small and large dimensions of the investigated items, high or low temperatures, inflammable or toxic substances, etc. At the same time the numerical solution may be obtained for the realistic conditions of the process under consideration which is not always possible within an experimental research [5].

The specified advantages as well intensive development of computers and numerical methods in the recent years allow to successfully use the modern CAE-systems, such as ProCAST, for mathematic simulation of the heat-and-mass exchange and fluid and gas dynamics which allows building the overall volume picture of the fluid flow and graphical visualization of the crystallization process, in particular: the fields of velocities, pressures or temperatures within the entire flow range.

ProCAST is the solution for computer simulation of all casting processes. The system is based on the finite-element method (FEM) which ensures the good accuracy of the description of the cast geometry and simulation model shape, considers the most of the thermal, crystallization, strain and deformation processes. This fact is repeatedly mentioned by the authors in their research papers [9], [10], [11], [12].

However, by analyzing their studies one may arrive at the conclusion that the use of the modern CAE-system ProCAST by mathematic simulation of the crystallization process detects the issues that may arise during

casting though against introduction of changes and achievement of the excellent result in the ProCAST system by the implementation of the results in practice the defects persist notwithstanding that they were absent in the mathematic model. This means that there is a necessity of creating one another stage – building of the analytical mathematic model.

The modern mathematics features the trend to identify the most relevant requirements to the mathematic models: universality characterizing the completeness of reflection of the real-life object properties by the model; adequacy – ability to represent the object properties with a tolerance not exceeding the set one; accuracy evaluated by the rate of coincidence of the real-life object properties and values of these properties obtained with the use of mathematic models.

Such models allow formulating the concepts for the efficient mathematic simulation of the process of structuring by crystallization. Dendrite crystallization represents an extremely complicated process related to the geometrical shape of dendrites, impurities diffusion, possible flow of melt within the interdendritic space, formation of the new nonmetallic phases (nonmetallic inclusions) and a number of other phenomena [13].

Melt crystallization is accompanied by a number of physical and chemical processes among which the following can be distinguished: processes affecting the melt composition; processes of origination and growth of a new phase at the crystallization front.

In order to consider such processes it is needed to build the mathematical model of melt crystallization that will allow determining in the analytical form the temperature distribution over the system, the law of the crystallization front motion and change of thickness of the liquid-crystal area appearing at the crystallization front.

It is known that the moving force of the crystallization process is the melt sub-cooling against the temperature T_φ of the equilibrium existence of the solid and liquid phases by the value ΔT:

$$\Delta T = T_\varphi - T_к = T_\varphi - T(y(t), t), \tag{1}$$

where $T_к = T(y(t), t)$ - the actual temperature of the crystallization front propagating according to the law $x = y(t)$ [14].

Presence of the temperature gradient and the supercooled melt before the crystallization front, dependence of the front temperature $T_к$ on the law of its motion and independence of origination of the crystallization centers results in instability of the plane crystallization front.

All of it is expressed in the growth of dendrites against crystallization and presence of the liquid-crystal area consisting of the crystallized dendrites oriented towards the direction of growth within the interdendritic space.

Formation of the dendrite structure is the result of the presence of this liquid-crystal area. The height of the liquid-crystal area determines the size of the cast structure grain.

It is convenient to use as a parameter of the liquid-crystal area Δy_0 the distance between the isotherms with temperatures $T_л$, T_c and T_φ:

$$\begin{aligned} \Delta y_0 &= y_л(T_л, t) - y_c(T_c, t), \\ \Delta y_c &= y(T_\varphi, t) - y_c(T_c, t), \\ \Delta y_л &= y_л(T_л, t) - y(T_\varphi, t), \end{aligned} \tag{2}$$

Where $T_л$, T_c and T_φ - temperatures of the alloy liquidus, solidus and beginning of crystallization of the leading phase [13].

It is needed to formulate and substantiate the basic assumptions required for specification of the mathematic model.

Taking into account that during the directed crystallization of the cast the wall thickness of the blade airfoil is significantly lesser than its length and the temperature gradient is directed along the vertical axis x it is possible to consider the process in one dimension as crystallization of semi-infinite space with the initial temperature $T_n > T_л$ [14].

Crystallization of the cast begins from the base of the ceramic mold that performs heat exchange through the mold box wall with the mold with the temperature T_0. The change of the liquid phase temperature during crystallization is determined by the thermal conductivity only. Where there is a stationary mold box it shall be believed that away from the crystallization front ($x \to \infty$) its temperature is constant and equals the initial one T_n. Where there is a movable mold box it shall be believed that the melt temperature maintains the constant value T_n at the distance l_0 away from the mold.

During the cast crystallization the ranges of the temperature variation of the liquid and crystal phases satisfying the conditions [14] are of major interest:

$$(T_{\Pi} - T_{\varphi}) / T_{\Pi} < 0,1 \div 0,2 \text{ and } (T_{\varphi} - T_{0}) / T_{\varphi} < 0,2. \quad (3)$$

Therefore, it can be considered that the thermal and physical parameters of the melt and solid phase do not depend on the temperature and are equal to the mean values within these ranges.

The specified assumptions are typical by solution of the crystallization tasks in terms of thermal conductivity with the use of analytical methods.

RESULTS

The diagram of the crystallization process with formation of a liquid-crystal area may be shown as intersection of the three domains indicated in the Fig. (**1,a**): $0 < x \le y_c(T_c, t)$ - solid phase, $y_c(T_c, t) < x < y_л(T_л, t)$ - liquid-crystal area, $x \ge y_л(T_л, t)$ - liquid phase [14].

It is apparent that the presence of the crystallization front with a random distribution of the dendrite formations heights indicated in the Fig. (**1, b**) excludes the possibility of analytical representation of solutions concerning the temperature distribution over the system. However, in this case a very complicated task of thermal conductivity for the internal part of the liquid-crystal area may be replaced through an easier task with equivalently equal heat sources and equal edge conditions. At the same time the solutions of the exterior problem for this domain are not changed. One may select as an equivalent problem the problem represented in the Fig. (**1, c**) with a fictitious plane crystallization front by introducing the equivalent heat instead of the specific melting heat *L*:

$$L = k_0 \cdot L', \quad (4)$$

Where $k_0 \ge 1$ considers the relative amount of the solid phase crystallized within the liquid-crystal area or level of the crystallization front development.

The derived solution will be true only for the domains $0 < x \le y_c(T_c, t)$ and $x \ge y_л(T_л, t)$ and the 1st approximation providing certain averaged distribution of temperatures within the liquid-crystal area [14]. At the same time at the moving plane boundary of crystallization there shall be additionally set the equation of the heat flux balance and temperature balance to a particular value T_φ. The temperature T_φ may either be of real physical significance – temperature of beginning of crystallization of the leading melt phase or represent a certain effective temperature.

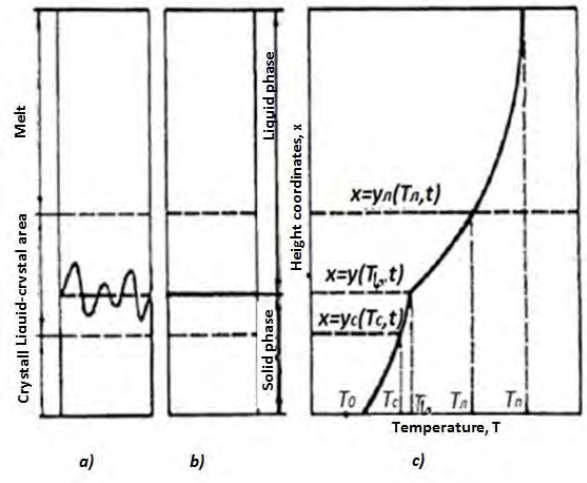

Fig. (3). Real-world (a) and simulation (b) diagram of the crystallization process and schematic distribution of temperature (c) over the cast height in the simulation diagram

However, in these two cases the law of motion of the fictitious plane crystallization front $x = y(T_\varphi, t)$ represents only motion of some isotherm with the specified temperature value since the real crystallization front features an extended surface due to the dendrites that have been formed.

DISCUSSION

The statement of the equivalent mathematic model for the first case (with a stationary mold box) takes the form:

$$\frac{\partial T_i}{\partial t} = a_i \cdot \frac{\partial^2 T_i}{\partial x^2}, i = 1, 2; \tag{5}$$

$$\lambda_1 \cdot \frac{\partial T_i}{\partial t} = a \cdot \left[T_1\ (x,t) - T_0 \right] \quad when\ x=0; \tag{6}$$

$$T_2(x,0) = T_{II}, T_2(x,t) \to T_{II} \quad when\ \ x \to \infty; \tag{7}$$

$$\lambda_1 \cdot \frac{\partial T_1}{\partial x} - \lambda_2 \cdot \frac{\partial T_2}{\partial x} = L \cdot \rho \cdot \frac{\partial y}{\partial t} \quad when\ x=y(t); \tag{8}$$

$$T_1(x,t) = T_2(x,t) = T_K = T_\varphi - \Delta T \quad when\ x=y(t); \tag{9}$$

$$\frac{\partial y}{\partial t} = k \cdot \Delta T, \tag{10}$$

where $i=1$ – solid phase with the variables domain $0<x\leq y(t),\ t>0$; $i=2$ – melt with the variables domain $x\geq y(t),\ t>0$; $y(t)$ - law of the crystallization front motion; k – kinetic parameter determining the rate of the grown-front velocity; ΔT – crystallization front subcooling against the equilibrium crystallization temperature T_e ;α – thermal resistance of the contact solid phase – ceramic shell mold – mold; T_0 – mold temperature; T_n – initial melt temperature; $L=k_0 L'$ – equivalent specific crystallization heat; L' – specific heat of melt crystallization; k_0 – coefficient considering the level of the crystallization front development; λ_i, α_i, p, c_i – thermal conductivity, thermal diffusivity, density and thermal capacity of the solid and liquid phases [14].

The stated boundary-value problem (5)-(10) belonged to the boundary Stefan's crystallization problems [15] and does not have an analytical solution for the entire crystallization cycle. That's why it is needed to consider different stages of reduction of the melt temperature at the boundary $x=0$ up to the onset temperature of crystallization and its behavior at low t as well as further behavior of the crystallization front in steady-state [14].

In order to get the solution of such boundary-value problem it is needed to use the self-similar solutions at the stage of the crystallization steady state according to which the equation of the crystallization front movement will take the following form:

$$y(t) = 2 \cdot \beta \cdot \sqrt{t}, \tag{11}$$

where β – parameter derived from the solution of the boundary-value problem.

CONCLUSION

Performing such mathematic simulation of the casting process with directed crystallization will allow developing the theoretical procedure for evaluation of grain of the cast structure and specify the basic requirements to the thermal and physical parameters of the process for the purpose of maintaining the cast structure stability and homogeneity since these conditions of formation of the cast solid during solidification thereof determine the performance properties of the aircraft engine critical parts.

As is known, the distance between the dendritic branches affects a lot of physic-mechanical properties of cast works, in particular, the yield point and tensile strength [2].

The life of the rotating blades, in its turn, depends on the casting manufacturing technology.

In this regard building of a mathematic crystallization model appears to be topical.

CONFLICT OF INTERESTS

The authors confirm that this article content has no conflict of interest.

ACKNOWLEDGEMENT

This work was supported by the Ministry of education and science of the Russian Federation in the framework of the implementation of the Program of increasing the competitiveness of SSAU among the world's leading scientific and educational centers for 2013-2020 years.

REFERENCES

[1] Krymov V. V., Yeliseev Y. S., Zudin K. I. Gas-turbine engine production / Edited by V. V. Krymov. M.: Mashinostroyenie / Mashinostroyenie – Polet, 2002. 376 p.

[2] Nyashina N. D. Mathematical model of dendrite crystallization of metal melt. Thesis work, Perm State Technical University – Perm, 2000. – 184 p.

[3] N. Saunders, M. Fahrmann and C.J. Small. The Application of CALPHAD Calculations to Ni-based Superalloys // Proc. Superalloys-2000. eds. K.A. Green, T.M. Pollock and R.D. Kissinger (TMS, Warrendale, 2000), 803.

[4] Modeling of Casting, Welding and Advanced Solidification Processes / M. Rappaz, M. Ozgu, K. Mahin (eds) (TMS Publ., Warrendale, PA, 1991), 836.

[5] Smirnov A. N., Kubersky S. V., Podkorytov A. L., Ukhin V. E., Kravchenko A. V., Orobtsev A. Y. et al. Continuous billet casting: Article thesis. – Donetsk: Digital publishing house, 2012. – 417 p.

[6] C.-A. Gandin, J.-L. Desbiolles, M. Rappaz, M. Swierkosz, Ph. Thevoz. 3D Modelling of Grain Structure Formation during Solidification // Supercomputing Rev. 8 (1996), 11-15.

[7] Y.-T. Kim, N. Provatas,N. Goldenfeld, J. Dantzig. Universal dynamics of phase-field models for dendritic growth // Physical Rewiew E, 1999, vol. 59. no. 3, 2546-2549.

[8] Tarabaev L. P., Yesin V. O. Formation of dendrite structure by directed crystallization of three-component alloys // Metals. 2001, No. 4. P. 39-45.

[9] Vdovin R. A., Smelov V. G. Design and optimization of the manufacturing process of casting the two-piece engine nozzles for the multi-functional core in the modern CAE-system ProCAST. Collected papers: XII Korolev's readings. International Youth Scientific Conference. – Samara, SGAU, 2013.

[10] Smelov V. G., Kokareva V. V., Malykhina O. N. Prospects of growth of the modern foundry production // Collected papers of the 16th International Scientific and Technical Conference of the Bryansk State Engineering Academy "New materials and technologies in machine engineering - 2012", 2012.

[11] V. V. Smirnov, S. P. Pavlinich, S. V. Bakerin, and A. M. Khairullina Use of PROCAST software to model casting systems for the centrifugal casting of GTE blades made of intermetallic alloys. Metallurgist, Vol. 57, Nos. 11–12, March, 2014 (Russian Original Nos. 11–12, November–December, 2013).

[12] Galkina N. V., Vdovin R. A. Development of the mathematical apparatus of crystallization of casts of the gas-turbine engine parts with account for formation of the shrinkage defects, cast porosity, thermal processes. Collected papers of the Students' Scientific and Technical Conference "Lukachev's readings", Samara, SGAU, 2014.

[13] Smirnov A. N., Makurov S. L., Safonov V. M., Tsuprun A. Y. Large-sized ingots. Article thesis. Donetsk National Technical University. – Donetsk, 2009. – 278 p.

[14] Golanov V. P. Managing the quality of manufacturing of gas-turbine engine blades by casting with directed crystallization. Thesis work. Samara State Aerospace University named after S. P. Korolev. - Samara, 2005. - 156 p.

[15] A. M. Meyrmanov; Editor-in-chief V. N. Vragov; AN SSSR, Siberian department, Institute for Hydrodynamics 238 illustrated 21, Novosibirsk, Nauka, Siberian department, 1986

ABOUT THE AUTHORS

Bogdanovich Valery Iosifovich, D. Eng. Sc., professor of faculty of the aircraft production and management of quality in machine engineering at the Samara State Aerospace University. The area of the author's expertise: plasma, plasma coatings, reactions rate, tailored ordered structures, heterogeneous processes, математическое mathematic simulation, reliability.

Golanov Vyacheslav Petrovich, candidate of engineering sciences, first deputy director general of the "Samara-Aviagaz" LLC. The area of the author's expertise: development of gas pumping units; production of the air and vacuum pumps; production of air and gas compressors.

Smelov Vitaly Gennadievich, candidate of engineering sciences, assistant professor of the department of the aircraft engine production at the Samara State Aerospace University, head of the laboratory for additive technologies. The area of the author's expertise: application of the CAD/CAM/CAPP-systems by training of specialists.

Nikolaeva Natalia Vladimirovna, post-graduate student of the the department of the aircraft engine production at the Samara State Aerospace University. The area of the author's expertise: foundry production of open-work parts with the use of additive technologies.