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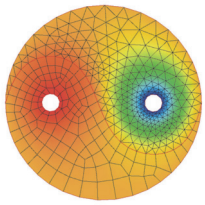

NUMERICAL DETERMINATION OF EQUIAXED GRAIN RADII ARISING IN THE CASTING DURING 3D SIMULATION OF SOLIDIFICATION

ROBERT DYJA, ELZBIETA GAWRONSKA*, ANDRZEJ GROSSER, PIOTR JERUSZKA, NORBERT SCZYGIOL

The Faculty of Mechanical Engineering and Computer Science, 42-201 Czestochowa, Dabrowskiego 69, Poland
**Corresponding author: elzbieta.gawronska@icis.pcz.pl*

Abstract

The knowledge of material structure allows to predict the mechanical properties of alloy casting. Such structure can be modelled in micro- and mesoscale. The first way is connected with alloy morphology and enables one to find out the shape of grains emerging during the solidification process. The second way allows to define the magnitude and distribution of these grains in the casting structure. Learning both of these ways greatly enhances one's knowledge about such mechanical phenomena as emerging stresses, strains, hot cracking and many others. This information makes it possible for one to predict the behaviour of castings during the cooling process or the further product exploitation. The one of the most difficult issues in the numerical and computer simulations of solidification is the modelling of the structure evolving in the casting. These simulations are extremely important in the work of an engineer in the foundry industry. The paper deals with a numerical modelling of equiaxed microstructure formation during the solidification of two-component alloys. The basic enthalpy formulation was applied to model the solidification. The equiaxed grain size depends on the average cooling velocity at the moment when the liquid metal reaches the liquidus temperature. The experimentally determined dependence between grain radius and cooling velocity was used in the calculation of average grain radii distribution.

Key words: grain radius, microstructure, casting, FEM, solidification modelling, computer simulation

1. INTRODUCTION

The cast products are characterised by the fact that their shapes and properties are formed when liquid metal is passing to the solid state. The casting solidification is a heterogeneous process, which means that solidification proceeds differently in every point of the casting. The change from the liquid to the solid state is a process composed of many physical phenomena. One of the most important ones is the microstructure formation. The microstructure formation is so important because it determines the usability values of sound castings and also influences the thermo-mechanical states in the solidifying and cooling castings. The casting microstructure is mainly composed of three zones of grains: equiaxed chill, columnar and equiaxed. The last one mostly has a dendritic structure. In many cases the microstructure of whole castings is composed only from equiaxed grains. This often occurs in non-ferrous metal castings.

The casting process is one of the most direct and shortest routes from a component design to a final product. This makes casting one of the major manufacturing processes, while making casting alloys some of the most widely used materials. One of the main reasons for the versatility of the casting process is the wide range of mechanical and physical properties covered by casting alloys. They may be of

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complex equipment and they are used in 90% of all manufactured goods (Stefanescu, 2001).

Solidification is an inherent part of the casting process. The structure of the casting is generated during the solidification and is also often the final structure of the casting. This in turn makes the mechanical properties of the casting, which are a direct consequence of the microstructure, controlled through the solidification process (Jamaly et al., 2015; Stefanescu et al., 2012). Solidification models often analyse solidification events at a micro-, a macro- and an intermediate scale – a mesoscale (Gawronska et al., 2016; Gawronska & Wodo, 2012; Gawronska & Wodo, 2013). The intermediate scale allows for the description of the microstructure features at grain level, without resolving the grain boundary. On this level solid-liquid interface appears in three regions: liquid, mushy (containing both liquid and solid phase), and solid. The macroscale is related to the (growing) solid phase as a whole and allows for the description of certain parameters such as the dimension of the grains or the extent zones of particular types of structures.

The casting solidification is a heterogeneous process, so it is different in each point of the casting. The course of the solidification can be described by a cooling curve or by a solidification curve – a curve between the liquidus and solidus lines in the phase diagram (see figure 1).

The first case describes the variation of the temperature within time and allows for the designate of the cooling rate at any time during the process. Whereas the second case is characterized by the quantitative changes of the part of solid and liquid phase in function of temperature. All possible solidification curves – describing changes of temperature during process (e.g. line no. 3 in figure 1) take place between two extreme cases i.e. equilibrium solidification (lever rule - line no. 1 in figure 1) and non-equilibrium solidification without back-diffusion (line no. 2 in figure 1). The first of them describes homogeneous distribution of solute concentration both when in liquid and solid phase of the casting. The second of them describes significant pushing out of solute to liquid phase and lack of diffusion of solute in solid phase. During the indirect solidification – between Scheil model and non-equilibrium solidification model (line no. 3 in figure 1 there is no alignment of the distribution of solute concentration in solid phase but there is a significant diffusion of solute. In the real castings, except for the rapidly solidifying layers adjoining to the mould and the slowly solidifying central areas of the massive castings, the indirect solidification occurs.

Numerical simulations are used for optimization of casting production. In many cases they are only possible technique for carrying out experiments whose real statement is complicated. Computer modelling allows defining the major factors for a quality estimation of alloy castings. Simulations help to investigate interaction between solidifying casting and changes of its parameters or initial conditions (Dyja et al., 2015a; Dyja et al., 2015b; Dyja et al., 2014). In order to achieve the efficient performance of large series of computational studies using reasonable resources, the framework needs to be not only accurate but also computationally efficient. Increasing capacity of computer memory makes it possible to consider growing problem sizes. At the same time, increase of the precision of simulations triggers even greater load. There are several ways to tackle this kind of problems. For instance, one can use parallel computers (Kim & Sandberg, 2012; Wyrzykowski et al., 2014), the other can use accelerated architectures such as GPUs (Michalski & Sczygiol, 2015) or FPGAs (Yang et al., 2012), and another can use special organization of computations (Gawronska & Sczygiol, 2010; Gawronska & Sczygiol, 2015; Ghoneim & Ojo, 2011).

In this paper we are concerned only with a part of the numerical modelling of thermo-mechanical phenomena occurring during the production of castings, i.e. the solidification and the formation of structure. We focus on the enthalpy formulation of solidification which is characterized by high efficiency in connection with the finite elements method (Date, 1994; Duan et al., 2002; Famouri et al., 2013; Ganguly & Chakraborty, 2006; Zienkiewicz & Taylor, 2000). We have described our own model of indirect solidification instead of the traditional models of equilibrium and non-equilibrium solidification (Sczygiol, 2000). We assumed that in the casting only one type of structure can be formed, namely the equiaxed structure. The grain size depended on the cooling rate. We carried out the numerical simulations of solidification for the alloy solidifying in the metal mould. The results are showed as distributions of the cooling rates and the average radii of the equiaxed grains. We have assumed the continuity boundary condition between the mould and the casting, while between the casting mould and the environment the Newton boundary condition has been assumed. We have transformed the equation describing the solidification into a system of algebraic

equations with the use of finite element method, Bubnov-Galerkin method and Green-Gauss theorem. After having done semi-discretisation and having got the equations consisting only of the time derivative, we have used one of the time integration schemes to get the results in which we were interested (Wood, 1990). We have also used parallel processing to assure effective time duration for simulations. During the implementation we have used TalyFem and PETSc libraries which allowed us to split structures such as matrices and vectors into many computing nodes (Balay et al., 2014; website about MPI, 2016; Kodali & Ganapathysubramanian, 2012; Wodo & Ganapathysubramanian, 2011).

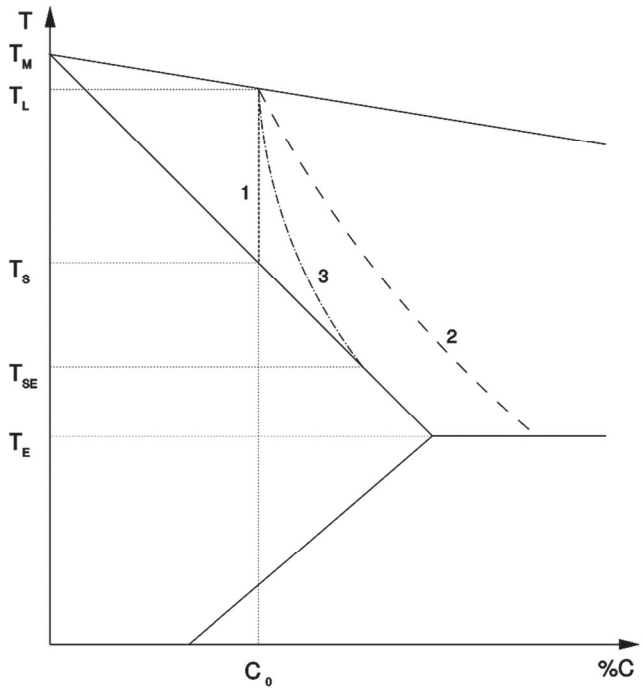

Fig. 1. *Models of solid phase growth in binary alloys (T – temperature, C –chemical composition of the alloy; T_M – solidification temperature of the base component (melt temperature), T_l – liquidus temperature, T_s – solidus temperature for equilibrium solidification T_{SE} – solidus temperature for indirect solidification).*

2. SOLIDIFICATION MODEL

Solidification is described by a quasi-linear heat conduction equation containing the heat source term, which describes the rate of latent heat evolution. The basic enthalpy formulation of this equation has the form

$$\nabla \cdot (\lambda \nabla T) = \partial H / \partial t \qquad (1)$$

where λ is the heat conductivity, in which the enthalpy is defined as

$$H(T) = \int_{T_{ref}}^{T} c\rho \mathrm{d}T + \rho_s L\big(1 - f_s(T)\big) \qquad (2)$$

where c is the specific heat, ρ is the density (subscript s refers to the solid phase, l would have denoted the liquid phase and f would have denoted the mushy zone), L is the latent heat of solidification and f_s is the solid phase fraction. Equation (1), with appropriate initial and boundary conditions, was solved by FEM. After semi-discretisation, modified Euler-backward scheme, in which the values of material properties are calculated on the basis of a known temperatures, was applied for integration over time. The final form of Eq. (1) after semi-discretisation and the application of the modified Euler-backward scheme, is as follows

$$(\mathbf{M}^n + \Delta t \mathbf{K}^n)\mathbf{T}^{n+1} = \mathbf{M}^n \mathbf{T}^n + \Delta t \mathbf{b}^{n+1} \qquad (3)$$

where **M** is the mass matrix, **K** is the conductivity matrix, **T** is the temperature vector and **b** is the boundary conditions vector. The superscript n denotes current time level and n+1 denotes next time level. Moreover, it is possible to directly take into account the forming microstructure in the above solidification model.

2.1. Models of solid phase growth

Solid phase growth is directly associated with the release of the latent heat of solidification, whereas the start and the end of this process is connected with the achievement of the liquidus and solidus temperature respectively (see figure1). For example, the binary alloy with eutectic transformation, for which the solidification model can be built, requires an appropriate numerical model of the solid phase growth. In the case of non-equilibrium solidification, described by Scheil equation, the eutectic temperature is always reached. This means that the final portion of metal solidifies at a constant temperature. In the equilibrium model of solidification, the final solidification temperature is dependent on the chemical composition of an alloy. Only for alloys with the solute concentration greater than their maximum solid phase solubility, the final solidification temperature is equal to the eutectic temperature. In the indirect solidification, the course of solidification depends on the path of solute diffusion, and thus on the size of grains in the casting structure. In turn, the average grain size is related to the cooling rate. The complete distribution of the solute in the liquid phase and its diffusion in the solid phase of the future grain assumes in the indirect solidification (figure 2).

The obtained solution connects the solute concentration on the solidification surface with the part of phase fraction. Next, using the relationship between concentration and temperature (phase diagram) a function binding the part of solid phase with temperature can be finally obtained. The mass balance of solute in the single grain area is

$$\begin{aligned} & m\eta^{m-1}(t)\frac{d\eta(t)}{dt}C_s(\eta(t),t) + \\ & + m\frac{1}{r_z}D_s\eta^{m-1}(t)\frac{dC_s(\eta(t),t)}{d\xi} + \\ & + \left(1-\eta^m(t)\right)\frac{dC_l}{dt} - m\eta^{m-1}(t)\frac{d\eta(t)}{dt}C_l(t) \end{aligned} = 0 \quad (4)$$

where subscript m is the grain dimension factor (m = 1 – planar grain, m = 2 – cylindrical grain, m = 3 – spherical grain), C is the solute concentration, η is the current thickness or radius of the solid phase grain, r_z is the final radius of the grain, D_s is the coefficient of the solute diffusion in solid phase and ξ designates the current coordinate. Since the equilibrium and nonequilibrium solidification models are extreme cases of the indirect solidification, the mass balance of solute in both instances can be obtained from Eq. 4.

By introducing the notion of a local solidification time t_f, the part of solid phase can be defined as (Sczygiol, 2000)

$$f_s = \sqrt{\frac{t}{t_f}} \quad (5)$$

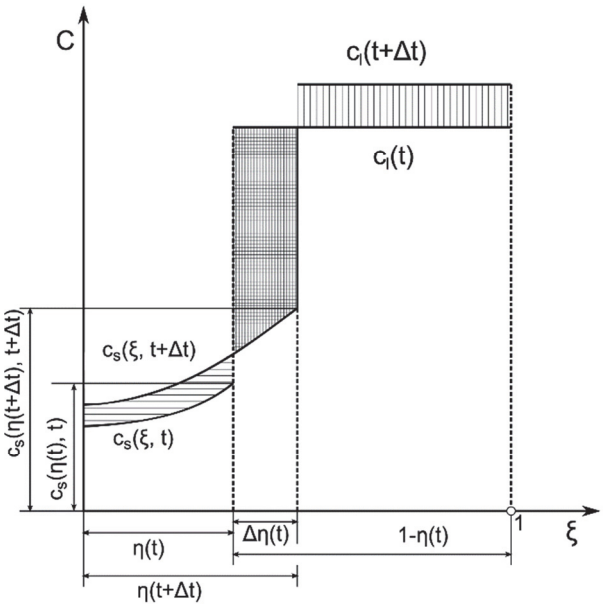

Fig. 2. *The momentary distribution of solute concentration in the grain.*

The Brody-Flemings equation for parabolic growth is (Sczygiol, 2000)

$$C_s = kC_0[1-(1-2\alpha k)f_s]^{\frac{k-1}{1-2\alpha k}} \quad (6)$$

where α is the dimensionless back-diffusion coefficient (vel Brody-Flemings coefficient), calculated as

$$\alpha = \frac{D_s t_f}{r_z^2} \quad (7)$$

the product $D_s t_f$ can be regarded as material parameter, and the solute partition coefficient is

$$k = \frac{C_s^*}{C_l^*} \quad (8)$$

wherein C^* designates the solute concentration on solidification surface.

By making additional assumptions (Ω – amendment of α coefficient) and necessary transformations Eq. 6 can be written as (Sczygiol, 2000)

$$f_s(T) = \frac{1}{1-2\Omega k}\left(1-\left(\frac{T_M-T}{T_M-T_l}\right)^{\frac{1-2\Omega k}{k-1}}\right) \quad (9)$$

where

$$\Omega(\alpha) = \alpha(1-\exp(-1/\alpha)) - 1/2\exp(-1/(2\alpha)) \quad (10)$$

If the numerical model of solidification assumes the possibility of forming the grains of different sizes and the solute concentration is lower than its maximum solubility in the solid phase, then, according to Eq. 10, a portion of grains can gain the eutectic temperature (in the part of casting which solidify at the latest) and another portion can solidify above that temperature during solidification process. It is crucial to the grain size in this case. If the solute concentration is equal to or larger than its maximum solubility in solid phase, then all grains gain the eutectic temperature.

2.2. Numerical model of equiaxed microstructure formation

The solidification process depends on the diffusion path length of solute and also on the grain size in the formatting microstructure in the indirect solidification model, the limits of which are determined by the equilibrium and non-equilibrium model. The indirect solidification model, in contrast to the non-equilibrium solidification model, allows the eutectic solidification to start at some solid phase fraction value, which depends on the grain dimension.

Numerical modelling of structure formed in the casting is one of the most difficult problems in com-

puter simulations of solidification. The extent of the zones of the different types of structure and the characteristic dimensions of the grains in these zones depend on the undercooling at the start of solidification. Undercooling, on the other hand, depends on the cooling rate. All the possible values of the cooling rates are between the infinitely large (T→∞) and infinitely small (T→0) value of the cooling rate.

Velocity of the grain growth in solid phase is an exponential function of undercooling (kinetic, curvature or constitutional) of liquid metal alloys. Velocity of the grain growth is (Stefanescu, 2001)

$$v = K(\Delta T)^n \tag{11}$$

where K is the alloy constant (obtained from measured solidification curves and the final grain radii in structure), $(\Delta T)^n$ – temperature change over time - is undercooling (and n takes value from 1.3 to 2.3, but is often equal to 1, too (Sczygiol, 2000). Assuming that only the equiaxed grains formed in the casting, the velocity of their growth can be written as

$$v = \frac{dr}{dt} \tag{12}$$

Substituting Eq. 12 to Eq. 11 and integrating in the range of 0 to r_z and of 0 to t_f, the final grain radius is

$$r_z = K(\Delta T)^n t_f \tag{13}$$

Since the maximum grain radius in structure is r_b, thus if $t_f \to \infty$ then $r_z \to r_b$, and if $t_f \to 0$ then $r_z \to 0$. In the paper it was assumed that only one type of microstructure is formed, namely equiaxed microstructure whose characteristic dimension is the final grain radius which depends on the cooling rate (Sczygiol, 2000)

$$r_z = r_b\left[1 - \exp(-1/\dot{T})\right] \tag{14}$$

where $\dot{T}$ is the average cooling rate calculated from the beginning of the process until the liquidus temperature is reached. It can be noticed that if $\dot{T} \to 0$ then $t_f \to \infty$ and $r_z \to r_b$; and if $\dot{T} \to \infty$ then $t_f \to 0$ and $r_z \to 0$. In Eq. 14 the maximum grain radius in the structure depends on the used casting alloy and it should be determined experimentally. For very large values of undercooling the fine-grain structure is obtained, in which the zone of frozen grains is. In the inner areas of the casting, where the undercooling is much lower and less differentiated than the undercooling of the layer in contact with the mould, the equiaxed grains radii are more or less the same and relatively large.

In the paper it was also assumed that the final grain radius depends on the cooling velocity of the liquid phase. This dependence was established experimentally for an Al-2%Cu alloy (Sczygiol, 2000).

3. RESULTS

An example of a computer simulation was carried out for Al-2%Cu alloy solidifying in a metal mould. This alloy was chosen because of its wide range of solidification temperatures (about 50 K). The finite element method to solve the enthalpy formulation of solidification supplemented by boundary conditions of continuity and Newton were used. The focus was on the indirect model of solid phase for binary alloys. The mesh contained the tetrahedral finite elements composed of 234988 nodes, of which 110321 nodes were in the casting. The assumed values of the material properties and the characteristic temperatures are taken from (Sczygiol, 2000; Sczygiol & Szwarc, 2001) and are presented in table 1.

Table 1. *Material properties*

	Liquid phase	Solid phase	Mould
ρ, kg/m^3	2498	2824	7500
c, J/kgK	1275	1077	620
λ, W/mK	104	262	40
L, J/kgK	390 000		
k	0,125		

The geometry of the casting-mould system is presented in figure 3, whereas the analysed casting together with the finite elements mesh is presented in figure 4. The external length, width and height dimensions of the mould are 240 mm x 75 mm x 75 mm, respectively. The physical model of the casting-mould system is shown in figure 5.

The continuity boundary condition with non-ideal contact between the casting and the mould was assumed. The conductivity of the separating layer was equal to 800 W/m^{2}K. The Newton boundary condition was established on the remaining boundaries. In the calculations the ambient temperature was equal to 300 K. The heat exchange coefficient with the environment was equal to 50 W/m^{2}K on the bottom boundary, and 100 W/m^{2}K on the other boundaries. On the boundary between the casting and the environment it was equal to 10 W/m^{2}K. The initial casting temperature was 960 K, while the initial mould temperature was 590 K.

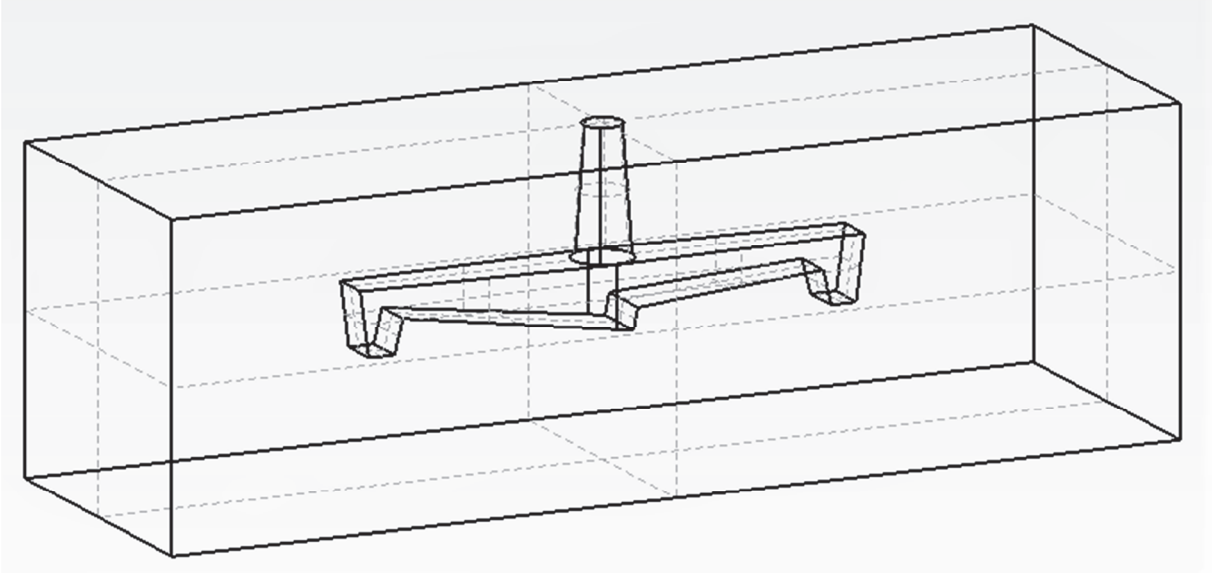

Fig. 3. *Geometry of the casting-mould system.*

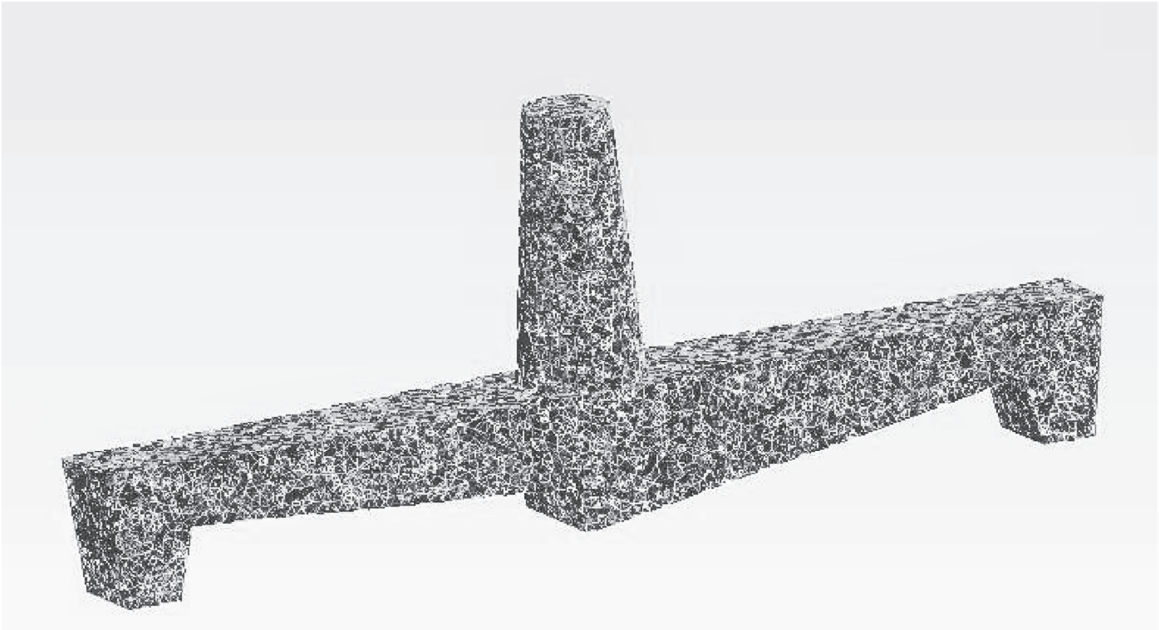

Fig. 4. *Analysed casting with the finite elements mesh.*

Fig. 5. *The physical model of the casting-mould system.*

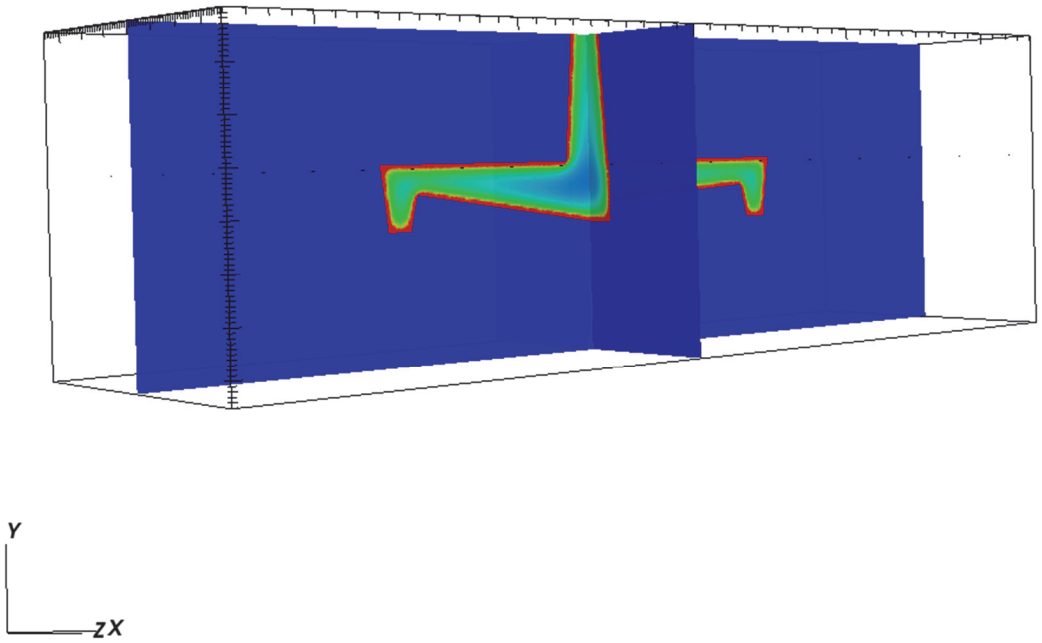

Fig. 6. *Distribution of the cooling rate (values calculated only for the casting – colour blue designates the smallest values, color red designates the largest values).*

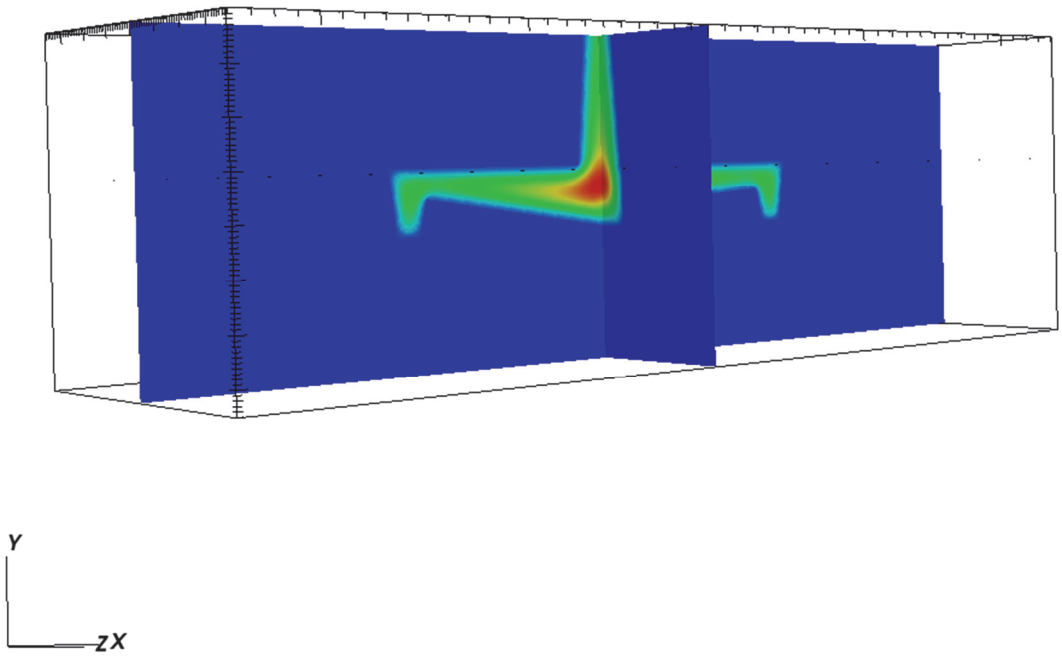

Fig. 7. *Distribution of the average final grain radii (values calculated only for the casting – colour blue designates the smallest grain radii, color red designates the largest grain radii).*

The results of computer simulation are shown in the following three figures (3D sliced view). Figure 6 shows the distribution of the average cooling velocity of the liquid phase. The calculated distribution of average final grain radii is shown in figure 7. The distribution of solid phase fraction at the moment when eutectic temperature (T_E) is reached and the eutectic solidification can take place, is shown in figure 8. It was assumed a linear variation of the thermal conductivity coefficient between the liquidus and solidus temperature. For the purpose of carrying out the numerical simulation, the required values of melt, liquidus, solidus and eutectic temperature were read from the phase diagram for Al-Cu and they are equal to $T_M = 933$ K, $T_L = 926$ K,

$T_S = 886$ K and $T_E = 821$ K respectively. In the calculations it was assumed that the maximal grain radius was $3.5 \cdot 10^{-5}$ mm (taken from experiment) and time step was equal to 0.025 s.

75 K/s), furthermore, because of the average grain radius being a function of the cooling rate, the substantial differences of grain size exist in the casting (see figure 7). The smallest grain radii, calculated at

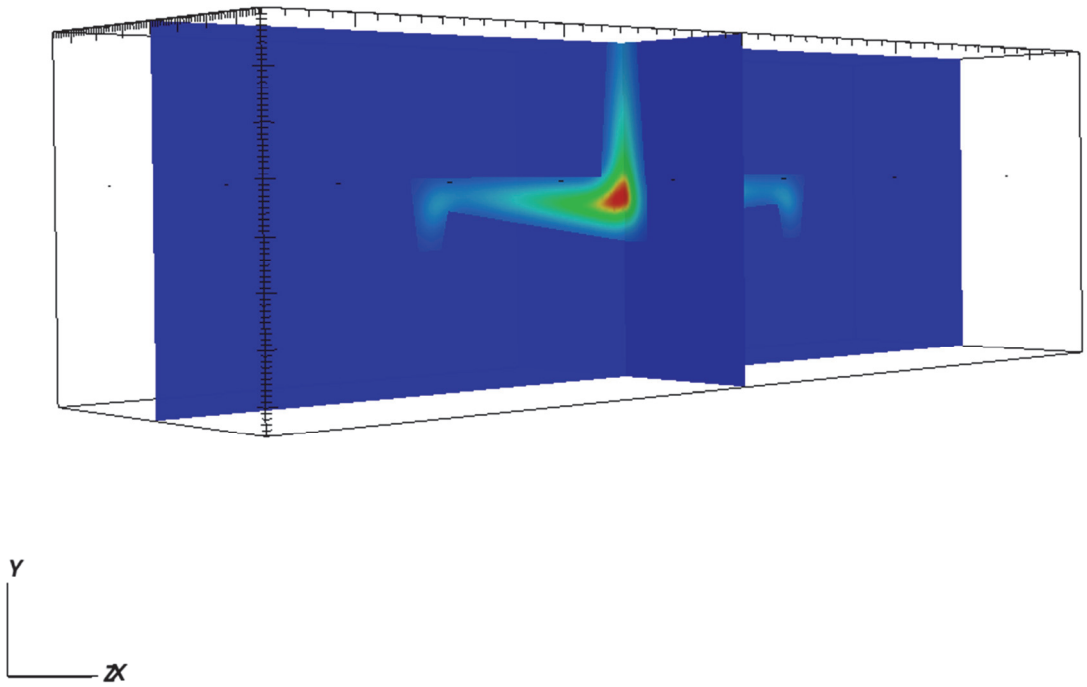

Fig. 8. *Distribution of the solid phase fraction (values calculated only for the casting – color blue designates the values nearly 1, color red designates the values slightly larger than 0).*

Solidification occurs the most rapidly in the nodes which are close to the contact walls of the casting and the mould (colour red in figure 6 – values of the cooling rate calculated only for the casting), what is more, the smallest grains arise there (colour blue in figure 7 – values of the grain radii calculated only for the casting). However, in the central part of the casting the solidification process occurs the slowest (colour blue in figure 6 – values of the cooling rate calculated only for the casting) and ends at the eutectic temperature. The distribution of the solid phase fraction in the moment when the eutectic temperature is reached illustrates diversity of solidification progress in various parts of the casting in the best way (see figure 8 – values of the solid phase fraction calculated only for the casting; colour dark blue presents the solid phase fraction which is nearly 1 and colour red presents the solid phase fraction which is slightly greater than 0). Because of the relatively large difference between the initial temperature of the liquid metal and the initial temperature of the casting, significant differences exist in the average cooling rate in the moment when the liquidus temperature is reached (the cooling rate changes in the range from almost 1360 K/s to almost

the nodes on the contact boundary between the casting and the mould, are almost 0.1515 mm. However, the largest grain radii, designated at the nodes in thermal centrum of the casting ie. in the area of the longest solidification, are almost 2.402 mm.

4. CONCLUSIONS

A new method of numerical modelling of equiaxed microstructure formation, based on the basic enthalpy formulation and the indirect solid phase growth model, has been proposed in this work. The indirect model, in contrast to commonly used non-equilibrium and equilibrium solidification models, makes it possible to take grain sizes into consideration in the calculation of temperature fields and solidification kinetics. The main advantage of the indirect solidification model is that the temperatures of the end of solidification, determined by this model, can cover the complete range from the equilibrium solidus temperature to eutectic temperature. Moreover, in this model the eutectic solidification can start at some solid phase fraction value, which depends on the grain dimension.

First of all, the applied model allows to determine the equiaxed grain radii in the castings made of two-component alloys. For the very large values of undercooling the fine-grain structure is obtained, including the zone of the frozen grain. In the inner area of the casting, where undercooling has a lower value nad is not greatly varied, the equiaxed grain radii are more or less the same and relatively large. Furthermore, the equiaxed grain size distribution is consistent with the real course of the process.

Numerical modeling has been developed to predict the solidification microstructure quantitatively in general and grain size in particular. Mechanical properties of castings depend on their microstructure. A model of equiaxed solidification, coupled with a macroscopic model for thermal description of solidification has been developed. The model is able to predict time-dependent thermal field and undercooling during the liquid and the solid phase growth. The relationship between grain radii and the cooling conditions were also investigated. The modeling was applied for calculation of the grain radii. It significantly enhances the understanding of solidification processing such as the behavior of solute Cu in aluminum alloys and the formed structure.

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NUMERYCZNE WYZNACZANIE PROMIENI ZIAREN RÓWNOOSIOWYCH POWSTAJĄCYCH W ODLEWIE PODCZAS 3D SYMULACJI KRZEPNIĘCIA

Streszczenie

Znajomość struktury materiału pozwala na przewidywanie właściwości mechanicznych odlewów. Taka struktura może być modelowana w mikro- i mezoskali. Pierwszy sposób związany jest z określeniem morfologii stopu i umożliwia znalezienie kształtu ziaren powstających podczas procesu krzepnięcia. Druga metoda pozwala określić wielkość i rozmieszczenie tych ziaren w strukturze odlewu. Znajomość obu tych sposobów znacznie poprawia wiedzę na temat takich zjawisk mechanicznych, jak pojawiające się naprężenia, odkształcenia, pękanie na gorąco i wiele innych. Informacje te pozwalają przewidywać sposób zachowania sie odlewów zarówno w trakcie procesu chłodzenia, jak i w dalszej eksploatacji produktu. Jedną z najtrudniejszych kwestii w symulacjach numerycznych i komputerowych krzepnięcia jest modelowanie struktury powstającej w odlewie. Symulacje te są niezwykle ważne w pracy inżyniera w przemyśle odlewniczym. W artykule przedstawiono numeryczne modelowanie struktury równoosiowej tworzącej się podczas krzepnięcia stopów dwuskładnikowych, w którym wykorzystano podstawowe sformułowanie entalpowe krzepnięcia. Wielkość ziaren równoosiowych uzależniono od średniej prędkości chłodzenia wyliczonej w chwilii, gdy ciekły metal osiąga temperaturę likwidusu. Do wyznaczenia rozkładu średnich promieni ziaren w odlewie wykorzystano zależność promienia ziarna od prędkości chłodzenia wyznaczoną na drodze eksperymentu.

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