The effect of the computed local solidification time on the material structure of solidified ceramics EUCOR

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Abstrakt Corundo-baddeleyit material (CBM) – EUCOR – is a heat- and wear-resistant material even at extreme temperatures. This article introduces a numerical model of solidification and cooling of this material in a non-metallic mold. The numerical model is capable of determining the total solidification time of the casting and also the place of the casting which solidifies last. Furthermore, it is possible to calculate the temperature gradient at any point and time, the local solidification time and determine the solidification interval of any point. The local solidification time is one of the input parameters for the cooperating model of chemical heterogeneity. This second model and its application on EUCOR samples prove that the applied method of measuring the chemical heterogeneity provides the detailed quantitative information on the material structure and makes it possible to analyze the solidification process. The analysis of this process entails statistical processing of the measurement results of the heterogeneity of the EUCOR components and performs the correlation of individual components during solidification. The verification of both numerical models was conducted on a real cast 350 x 200 x 400 mm block.

1 Introduction

The corundo-baddeleyit material (CBM) belongs to the not too well known system of the Al_2O_3-SiO_2-ZrO_2 oxide ceramics. Throughout the world, it is produced only in several plants, in the Czech Republic under the name of EUCOR – Prospectus EUCOR [1]. It was shown by Ticha at al. [2] that from the foundry property viewpoint, EUCOR has certain characteristics that are similar to the behavior of cast metal materials, especially steel for castings – Khvorinov [3]. The information relating to the properties of EUCOR is covered in publication Stransky at al. [4] and Kavicka at al. [5]. EUCOR castings can also be made with a riser – to a certain extent in a similar way as pouring steel for castings.

2 The assignment and preparation

The assignment focussed on the investigation of the transient 3D temperature field of a system comprising a casting-and-riser, the mold and ambient, using a numerical model. The dimensions of the casting — the so-called ‘stone’ — were 400 x 350 x 200 mm (**Fig. 1**). The initial temperature of the mold was 20°C. The pouring temperature of the melt was 1800°C. That was approximately 300°C higher, when compared with, for example, the steel pouring temperature. The temperature of the liquidus was 1775°C and the solidus 1765°C. **Fig. 2** shows the network for the original casting, riser and mold.

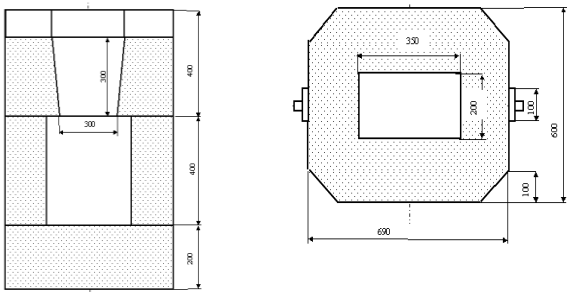

Fig. 1 The casting-riser-mold system

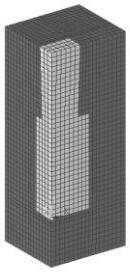

Fig. 2 The 3D network of the system with the original riser

The Fourier equation describes the transient temperature field in a mold. Here, it is necessary to introduce the specific volume enthalpy $h_v = c.\rho.T$, which is temperature dependent. The thermodynamic enthalpy function includes also latent heat of the phase or structural changes. The equation then takes the following form:

$$\frac{\partial h_v}{\partial \tau} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \tag{1}$$

The specific heat capacity c, density ρ and heat conductivity k are also temperature functions. The explicit difference method had been chosen for the solution of both equations. The program also considers the dependence of the heat-transfer coefficients (on all boundaries of the system) on the surface temperature. Software ANSYS integrates an original mesh generator.

3 Measurements and computation results. Optimization of the riser

The numerical model of the temperature field of the casting was confronted with the experimental measurements and corrected. The temperatures were measured in the actual casting and also in the mold.

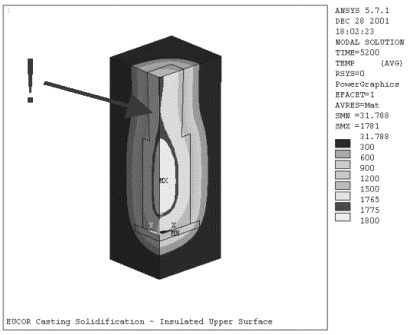

Fig. 3 The temperature field of the system comprising the casting, the original riser and mold at 5200s

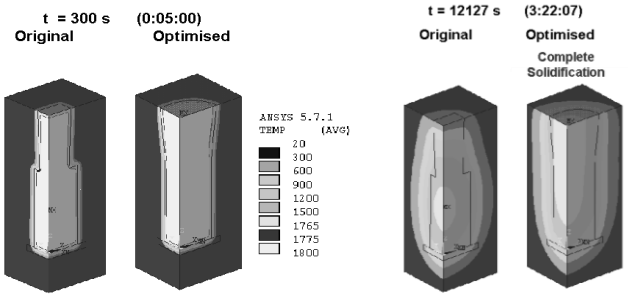

Fig. 4 The temperature fields before and after optimization (300 s and 12127 s after pouring)

The directed solidification with the original riser was not achieved because the riser was 'frozen' 5200 s after pouring (**Fig.3**). The new shape of the riser was selected according to the latest findings. After several modifications, the application with an optimized riser ensured the directed solidification. **Fig. 4** compare the temperature fields of the casting and riser inside the mold at 2 points in time — from the pouring into the mold to the total solidification. The casting with the new riser has the directed solidification — the casting was still being refilled from the riser.

4 The model of the chemical heterogeneity and its application

The concentration distribution of individual oxides, making up the composition of the ceramic material EUCOR, was determined using an original method developed by Dobrovska at al. [6] and applied in the process of measuring the macro- and micro-heterogeneity of elements within ferrous alloys. This method was initially modified with respect to the differences occurring during solidification of the ceramic material, when compared to ferrous alloys. It was presumed that within EUCOR, the elements had been already distributed, together with oxygen, at the stoichiometirc ratio (i.e. the chemical equation), which characterized the resulting composition of the oxides of individual elements after solidification. The preconditions for the application of the model of chemical heterogeneity on the EUCOR material are as follows:

If the analytically expressed distribution of micro-heterogeneity of the oxides of the ceramic material is available, if their effective distribution coefficient is known, and if it is assumed that it is possible to describe the solidification of the ceramic material via analogical models as with the solidification of metal alloys, then it is possible to conduct the experiment on the mutual combination of the calculation of the temperature field of a solidifying ceramic casting with the model describing the chemical heterogeneity of the oxides.

If the Brody-Flemings Model [7] is applied for the description of the segregation of oxides of the solidifying ceramic material and if an analogy with metal alloys is assumed, then it is possible to express the relationship between the heterogeneity index I_H of the relevant oxide, its effective distribution coefficient k_{ef} and the dimensionless parameter α using the equation

$$[\ln(2\alpha k_{ef})]/(1 - 2\alpha k_{ef}) = \{\ln[(1 + nI_H^{(m)})/k_{ef}]\}/(k_{ef} - 1) \quad (2)$$

the right-hand side of which $\{\ln[(1+ nI_H^{(m)})/k_{ef}]\}/(k_{ef}- 1)$, based on the measurement of micro-heterogeneity, is already known and through whose solution it is possible to determine the parameter α, which is also on the right-hand side of the equation in $2\alpha k_{ef}$. The quantity n has a statistical nature and expresses what percentage of the measured values could be found within the interval $x_s \pm ns_x$ (where x_s is the arithmetic mean and s_x is the standard deviation of the set of values of the measured quantity). If n = 2, then 95% of all measured values can be found within this interval.

If the dimensionless parameter α is known for each oxide, then a key to the clarification of the relationship exists between the local EUCOR solidification time θ, the diffusion coefficient D of the relevant oxide within the solidifying phase and the structure parameter L, which characterizes the distances between individual dendrites (in steels) or cells (in ceramics). The equation of the dimensionless parameter α (Fourier´s number for mass transfer) is

$$\alpha = D\theta/L^2 \quad (3)$$

It is possible to take the dimension of a structure cell as the structure parameter for the EUCOR material. The verification of the possibility of combining both methods was conducted on samples taken from the EUCOR blocks – from the edge (sample B) – and from the centre underneath the riser (sample C). Both the measured and the computed parameters of chemical micro-heterogeneity and the computed parameters of the local solidification time θ (according to the temperature-field model) were calculated. The local solidification time of the sample B was θ_B = 112.18 *s* and of the sample C was θ_C = 283.30 *s*. The very close values of the parameters $\alpha/\theta = D/L^2$ of the seven analyzed oxides of elements Na, Al, Si, K, Ca, Ti, and Fe $D/L_B^2 = (6.51\pm0.25).10^{-4}$ and $D/L_C^2 = (2.45\pm0.12).10^{-4}$ [1/s] indicated that the redistribution of these oxides between the melt and the solid state ran in a way, similar to that within metal alloys,

namely steels. The average value of D = (2.07±0.11) x 10^{-6} cm^2/s. For these cases it was possible to get the magnitude of the structure parameters that governed the chemical heterogeneity of the values

$L_B=\sqrt{[(2.07 \times 10^{-6})/(6.51 \times 10^{-4})]}=0.05639$ and $L_C=\sqrt{[(2,07 \times 10^{-6})/(2.45 \times 10^{-4})]}=0.09192$ [cm]

The comparison of the micro-structures of the analyses samples B and C (**Fig. 5 and 6**) has clearly shown that the sample B micro-structure (L_B) was significantly finer than the micro-structure of the sample C (L_C). The sample B structure in **Fig. 5** characterizes higher cooling velocity of the EUCOR material from the solidus temperature, when compared with the structure C in **Fig. 6**. The higher diameter of the structure parameter *L* corresponds to the lower cooling velocity of the same material.

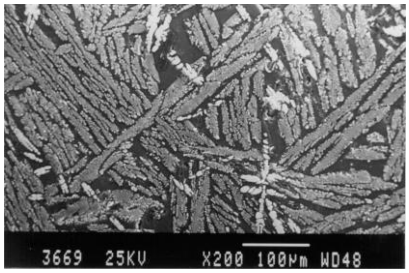

Fig. 5 The structure of the sample B (L_B = 564 µm)

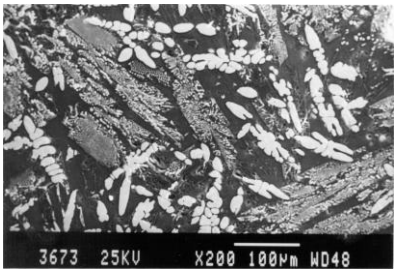

Fig. 6 The structure of the sample C (L_C = 919 µm)

5 Conclusions

This paper discusses the numerical model of the transient temperature field and the numerical model of the chemical heterogeneity, their application and combination. The combination of both models makes it possible to estimate the structure parameter, which expresses the size of the crystallites of the resultant material structure.

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