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Prediction of useful casting structure applying Cellular Automaton method

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Abstract

The results of simulation investigations of primary casting's structure made of hypoeutectic Al-Si alloy using the Calcosoft system with CAFE 3D (Cellular Automaton Finite Element) module are presented. CAFE 3-D module let to predict the structure formation of complete castings indicating the spatial distribution of columnar and equiaxed grains. That simplified model concerns only hypoeutectic phase. Simulation investigations of structure concern the useful casting of camshaft which solidified in high-insulation mould with properly chills distribution. These conditions let to apply the expedient locally different simplified the grains blocs geometry which are called by the authors as pseudo-crystals. The mechanical properties in selected cross-sections of casing are estimated.

Keywords: Structure modelling, Solidification, Cellular Automaton, Al-Si alloy

1. Introduction

One of the most significant casting's feature is the natural locality of mechanical properties attributed to structure variation being the result of solidification process. Variation of thermal conditions of mould influence on the casting e.g. chills applying which enable to obtain the proper temperature gradient allowing the columnar zone formation which locally could carry higher operating mechanical weights. It is necessary to control this gradient and also structure gradient and its mechanical properties of casting in order to in optimal way use the casting's properties of this specific *in-situ* composite. Extremely helpful in this case is computer simulation of foundry process which let to predict the oriented structure zone occurrence. This zone has the expected higher local mechanical properties. Only few simulation systems let to structure prediction of complete castings taking into consideration the zones of structure. They are based on "hard modelling" [1]. Mostly the crystallization simulation process is limited to single grain or groups of equiaxed grains in dimensionally limited domain.

Micro model responsible for structure prediction according to crystallization phenomena is elaborated and formally validated only in few foundry simulation systems e.g. Calcosoft. ProCAST system contains some modules from Calcosoft pretends to be admit as the best simulation system.

In world foundry there is only small number of factories which use that system. It can't be still equal to Magmasoft system [2]. However Simtec system finds recognition in some German foundries and in opinion of its authors achieves successes [16].

It should be pointed the Magma-iron module in Magmasoft system. It enables the crystallization modelling based on empirical relations ("soft modelling" [1]) which consider the active nuclei formation rate of crystallizable phases (austenite and graphite) and afterwards from these nuclei the growth rate in function of local undercooling (different for particular cells – meshing) of alloy zone which are between liquidus and solidus temperature). Similar model is valid in this system to pearlite transformation. It should be pointed that above mentioned relations require empirical parameters knowledge adapted to alloy type and its cooling

intensity. The Magma-iron was elaborated and introduced to iron castings only. It is still in progress the similar micro model for aluminum alloys.

Prediction of useful casting structure should be combined with the reliable level to accurate results. Firstly it should be made the validation of selected system using simple castings to estimate the influence of particular parameters available in system's data base in other words so called model's sensitivity. Afterwards it should be focused on utility castings. That kind of test was made in this paper.

2. Microstructure formation model and its validation

In simulation tests it was used the CAFE (Cellular Automaton Finite Element) model of Calcosoft system. This system is available in 2-D and 3-D version. In this work it was made the structure prediction using 3-D version. This model let to model the structure of geometrically simple blocs (without secondary dendrite arms) according to complete castings where the columnar and equaiaxed crystals are formed. This model assumes that in structure of hypoeutectic alloy appears α - phase only. Modelling is based on coupling heat transfer (finite element method, thermal model based on Fourier-Kirchhoff equation) with cellular automaton method (empirical model) which is used to describe nucleation process according to Gauss distribution and grain growth based on KGT (Kurz, Giovanola, Trivedi) model [4,5]. This model was described in detailed in the papers of system's authors [5-9] and authors of this paper [11-15].

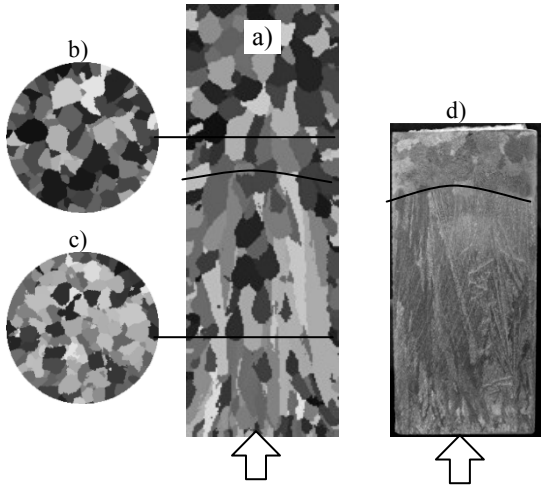

Fig. 1. Example of structure prediction: a – virtual cylindrical casting ϕ30 mm and d) real cross-section (etch: F5S20A20); transverse cross-sections in the distance from cooled bottom of casting: b) 60 mm, c) 20 mm, d) real cast structure. Arrows indicate chills location.

In the previous papers the necessary validation of Calcosoft CAFE was made. Investigations were carried out on cylindrical castings. Two dimensions of casting were used: ϕ30 and ϕ70 mm intensively chilled from one face. The experimentally-simulation validation with CAFE model sensitivity studies was made. It let to define the influence of selected values parameters of thermal model (FE) and empirical model (nucleation and growth) on the location of columnar-to-equaiaxed transition zone (CET), grain size (columnar, equaiaxed) and angle of columnar crystals according to vertical casting axe. The example of structure prediction for ϕ30 mm casting validation was shown in fig. 1.

On this basis it was elaborated the instruction to structure prediction for aluminum alloys in wide range of value parameters for thermal and empirical (structural) models.

3. Example of CAFE model exploited to casting structure and properties prediction

The test of structure prediction for useful camshaft casting was realized (fig.2). Real process prediction especially structure formation has sense when the useful castings are labored while not only simple shape benchmark castings which have shape of simple solids and could be related under some conditions to more complicated one. This is the reason why it was decided to predict the structure of useful casting. It is necessary to accomplish requirements of local mechanical properties resulting from exploitation conditions.

Simulation investigations were carried out according to constructor assumptions for AlSi7Mg alloy casting which solidified in high-insulation mould with chills. The geometry of casting is certainly complex according to investigations which were carried out in previous papers [11-14] concerning cylindrical ϕ70 and ϕ30 mm test castings.

According to locality of mechanical properties of this casting it was admitted by constructor that it should has in cam part and on the faces (there will be face gear teeth cutting) higher local mechanical properties according to exploitation requirements. Application of chills (one curvature shape chill) let to force structure orientation (direct solidification) i.e. formation of columnar dendrites in these key locations. Application of structure prediction method based on CAFE 3-D model let to specify location of columnar-to-equaiaxed zone transition (CET) and grain size in particular places of casting. On that base in these key locations there were the mechanical properties estimated.

Thermal parameters and parameters useful in nucleation and growth model in virtual investigations were taken from best fitted of structure for ϕ70 mm cylindrical casting (look investigation [16]) which solidified in high-insulation mould with chill. The optimal values parameters were shown in table 1.

Virtual structure of camshaft casting on the longitudinal and on key selected transverses cross-section were shown in fig. 2 (CET zone location were shown there too). Values parameters of structure description were shown in table 2.

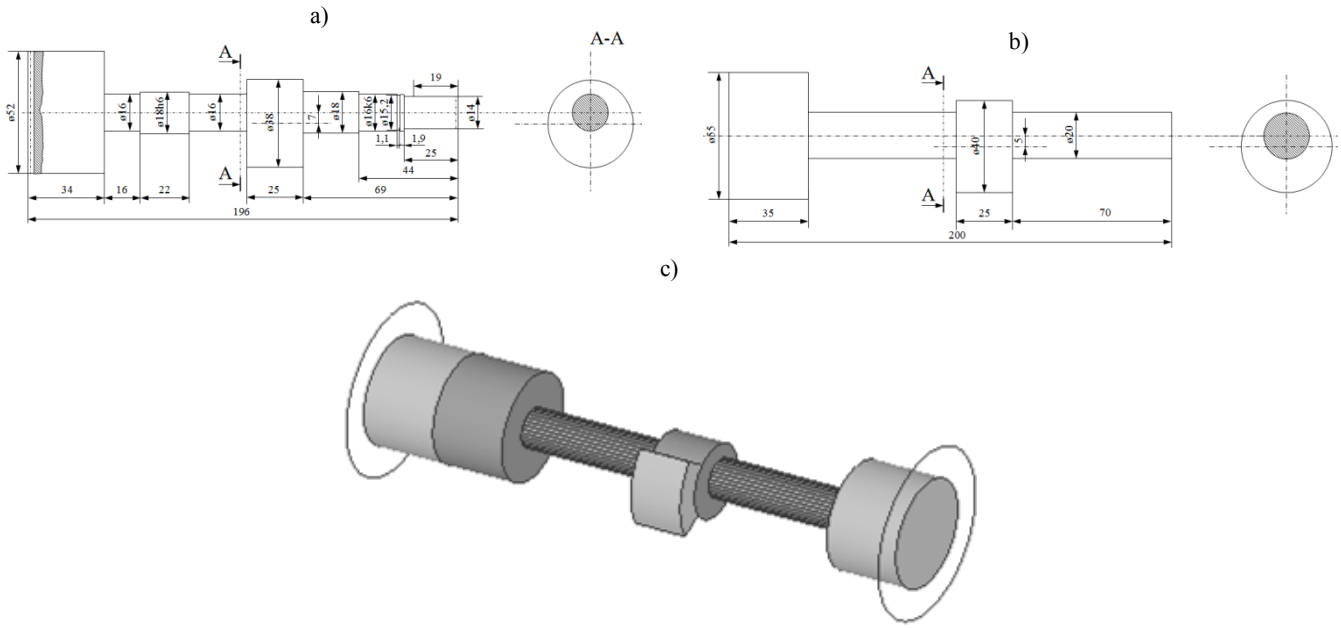

Fig. 2. Camshaft drawing: a) construction, b) raw casting, c) 3-D casting CAD geometry (with chills)

The results of virtual structure parameters (grain size) let to estimate the mechanical properties in particular four zones of casting (look to fig. 3 and table . 2). Values of these properties were shown in table 3. Correlation of structure parameters and local mechanical properties of casting was based on available and reliable for tested alloy data taken from experiment which was made and described in the work by our team [16]. Because of methodology adopted in this paper the camshaft casting need to be divided on the four selected zones.

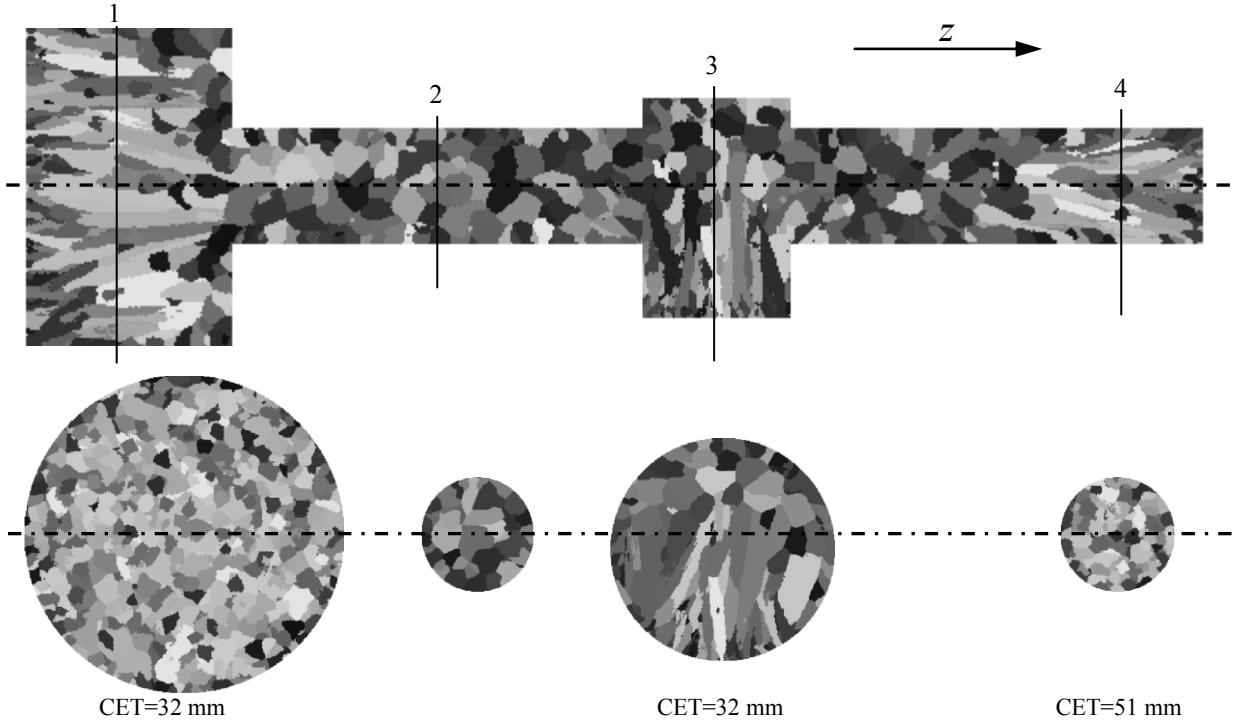

Fig. 3. Camshaft casting structures which solidified in high-insulation mould with chills

Table 1.
Optimized values parameters applied to simulation tests based on [15]

Parameter	Name		Value	Unit
Parameters of thermal model (FE)				
λ_{HI}	mean heat conduction of high-insulation mould		0,5	W/mK
C_{pHI}	mean heat capacity of high-insulation mould		587	kJ/m^{3}K
λ_{Ch-Cu}	mean heat conduction of copper chills		390	W/mK
C_{pCh}	mean heat capacity of copper chills		3300	kJ/m^{3}K
λ_{AlSi7}	mean heat conduction of alloy	liquid phase	90	W/mK
		solid phase	130	
$C_{p-AlSi7}$	mean heat capacity of alloy	liquid phase	3483	kJ/m^{3}K
		solid phase	2700	
L_{AlSi7}	latent heat of AlSi7 alloy		$1131 \cdot 10^9$	J/m^3
$\alpha_{cast-mould}$	mean heat transfer coefficient on cast-mould bound		10 000	W/m^{2}K
$\alpha_{cast-chill}$	mean heat transfer coefficient on cast-chill bound		2500	W/m^{2}K
$\alpha_{mould-amb.}$	mean heat transfer coefficient on mould-ambient bound		20	W/m^{2}K
T_{Al}	melting temperature of pure Al		660	°C
T_{eut}	Al-Si eutectic temperature		572	°C
c_0	initial solute concentration (Si)		7	%
k	partition coefficient		0,117	*non-dim.*
m	liquidus slope		-6,85	°C/%
Parameters of empirical model of crystallization (CA)				
ΔT_{m-s-HI}	undercooling (high-insulation mould surface)		5	K
ΔT_{m-s-Ch}	undercooling (chill surface)		10	K
ΔT_{m-v}	undercooling (bulk of liquid)		2	K
n_{s-HI}	nucleation density (high-insulation mould surface)		$1 \cdot 10^5$	1/m^2
n_{s-CH}	nucleation density (chill surface)		$8 \cdot 10^5$	1/m^2
n_v	nucleation density (bulk of liquid)		$8 \cdot 10^6$	1/m^3
$\sigma_{\Delta Ts-HI}$	standard deviation (high-insulation mould surface)		0,4	K
$\sigma_{\Delta Ts-Ch}$	standard deviation (chill surface)		0,4	K
$\sigma_{\Delta Tv}$	standard deviation (bulk of liquid)		0,4	K
a_2	growth kinetics coefficient (1)		$2{,}9 \cdot 10^{-6}$	ms^{-1}K^{-2}
a_3	growth kinetics coefficient (2)		$1 \cdot 10^{-9}$	ms^{-1}K^{-3}

Table 2.
Structure parameters (look. fig. 3)

Cross-section location / CAFE structure parameter	Virtual structure			
	Z=17 mm	Z=70 mm	Z=117 mm	Z=188 mm
Total grains number (Nb)	598	50	164	120
Grain density on the surface, $1/m^2$	256787	160148	148777	384356
Mean grain surface, $F_{z\,śr.}$, mm^2	3,89	6,24	6,72	2,6
Mean grain size $d_{z\,śr.}$, mm	3,64	3,62	3,46	2,9

Table 3.
Estimated mechanical properties for particular casting's zones

Camshaft segment no	Mechanical properties		
	R_m MPa	$R_{0,2}$ MPa	A1 %
1	148	105	~12
2	126	79	~5
3	156	102	~14
4	162	97	~16

4. Summary

Before starting of useful casting (usually quite complex shape) structure prediction it is necessary to check in the first place model validation state of the simulation system. The best solution is to precede that procedure by the use of model sensitivity tests on particular parameters values changing for simple casting shape. Afterwards those results should be adapted to more complex castings simulation tests.

On the basis of the realized simulation investigations using structure prediction algorithm (Calcosoft CAFE 3-D system) for camshaft casting it can be stated that this model let to, in satisfactory way, determine the CET zone location, grain size and orientation of grains in different zones of casting influenced by moulding technology with the use of chills [15].

The CAFE model can be successfully applied for complex castings that is unquestionable trump in it's disseminate to apply in industrial conditions. It shouldn't be assumed that verified validation tests of this model for simple shape castings (cylindrical and plate castings) are needless according to other industrial castings. On the contrary it should concern especially of shift the predicted local structure parameters to local mechanical properties with the use of miniature trepanned sample allowed by European and ASTM standard.

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