THE PROBLEMS OF TESTING AND VALIDATION OF THE CELLULAR AUTOMATON-FINITE ELEMENT METHOD APPLIED TO FORECASTING A MICROSTRUCTURE OF HYPOEUTECTIC Al-Si ALLOYS

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SUMMARY

The work provides description of modeling with the use of the Cellular Automation-Finite Element Method and its testing, connected with an attempt of validation of the Calcosoft System (CS-CAFE). Results of identification of selected parameters used in stochastic and thermal models are provided, inclusive of determining their effect on the results of forecasting geometric parameters of hypoeutectic Al-Si microstructure alloys. Validation has been carried out with a simulation-experiment method under various conditions of thermal interaction with the casting mould. The results of metallographic studies of structure of specially made castings have been used.

Keywords: microstructure, validation, cellular automaton, modeling, Al-Si alloys

1. INTRODUCTION

Modelling of the phenomena accompanying formation of metal alloys structures, aimed at virtualization, is related to the change in their state of transformation from liquid to solid (casting and solidification processes). According to physical conditions of the crystallization process, the modelling was initially developed based on deterministic models, describing nucleation and growth only of equiaxial (globular)

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crystals. The models are characterized using many simplifications and limitations, referred to, among others, in [2]. This was one of the reasons for developing stochastic (probabilistic) methods.

The modelling process was, first of all, developed on the grounds of the Monte Carlo method [1, 5, 9]. A fault of the method consists in the lack of connection between kinetics of the growth of crystal with undercooling at the solid–liquid interface, e.g. in the form of a relationship between growth rate of dendrite tip and local undercooling [9]. Moreover, compatibility of the time step applied for the computation purposes and the real time remains ambiguous. Thus, the mechanism of grain growth used in solidification models based on the Monte Carlo method does not satisfactorily reflection of the physical process [3]. A promising method of microstructure modelling, or even considered as the best one, developed since 1992, is the method based on the so-called cellular automaton. The method consists in preliminary discretization of the casting – the finite element method – of English abbreviation FE (heat transfer modelling) and secondary meshing of the space subject to modelling, leading to creating the cells of very small dimensions, below 1 millimeter (modelling of the phenomena accompanying formulation of the structure by means of Cellular Automaton - CA). Therefore, the method is signed as CAFE. At present the method is widened by solidification model (FT) [4] that allows for bilateral referencing of the nodes in all domains of the casting: the mesh of cellular automaton and finite element mesh, in order to ensure well defined solidification front, considered as the liquid-solid interface.

2. SCHEMATIC DESCRIPTION OF THE CELLULAR AUTOMATION - FINITE ELEMENT MODEL

The Calcosoft 2D system with the CAFE module is a tool for modelling formation of a pseudodendritic structure. This deterministic-probabilistic model is supported on clearly defined physical bases and, therefore, may reflect, at least qualitatively, e.g. the effect of cooling or concentration rate of the C solute on its microstructure. As it was mentioned above, the method consists in joining the calculation related to heat transfer carried out with the finite element method with cellular automaton, thus allowing to describe the nucleation mechanisms and the growth of dendritic grains (Fig. 1).

The CAFE module assumes that nucleation may occur near the mould surface and in the bulk of liquid (inside of casting), in accordance with two \( \text{à priori} \) assumed nucleation intensity functions that are to be activated during the simulation, upon their local undercooling. Grain density (number) \( n_s \) arising while \( \Delta T \) undercooling at the mould surface and \( n_v \) – in bulk of liquid is calculated through integration of Gaussian curve (Fig. 2a). The nucleus \( n_v \) arising this way (Fig. 2b) grows during a given time step to the size of a new grain \( V \). Main crystallographic directions \([10] \) and \([01] \) of the growing nucleus make the angles \( \theta \) and \( \theta + \pi/2 \) with the horizontal axis of the CA mesh, respectively. A nucleating cell, on the grounds of an assumption, has homogeneous temperature and is surrounded by four adjacent cells marked by \( \mu_1, \mu_2, \mu_3, \mu_4 \) (Fig. 2b) [3]. It was also assumed that dendritic mesh \( n_v \) of the cell evolves as a square-shaped
shell. Four semi-diagonals (j=1 to 4) of the square correspond to the growth directions of dendrite tips (in 2D). The distance $L_{v,j}$ between the plane $<11>$ and middle of the cell is described by the relationship [3]:

$$L_{v,j}^t = L_{v,j}^{t-\delta t} + u_{\Delta T_{v,j}} \cdot \delta t$$

(1)

where:
- $\delta t$ – time step; in the CA model it must satisfy the condition $\delta t \leq \delta t_{\text{max}}$: ($\delta t_{\text{max}} = L/v_{\Delta T_{\text{max}}}$),
- $v_{\Delta T_{\text{max}}}$ - tip growth rate of the biggest dendrite, i.e. for maximal undercooling,
- $L$ - cell length (CA),
- $u_{\Delta T_{v,j}}$ - dendrite tip growth rate resulting from calculation of temperature field (local undercooling, cf. Fig.7).

Fig. 1. Description of modelling scheme of dendritic structure formation with application of the CS CAFE-2D model: a) present state, b) version with FT mesh (Front Tracking mesh) using [3,4].

Rys.1. Schemat modelowania powstawania struktury dendrytycznej z zastosowaniem metody CS CAFE-2D: a) stan obecny, b) wersja z użyciem siatki FT (ang. Front Tracking mesh) [3,4].
Experimental tests have been carried out with cylindrical castings of 30 mm diameter made of non-modified AlSi9 alloy, in a silica sand mould and in high insulating (microsphere) mould, containing a chill - D (Fig. 3a). Parameters of the microstructure obtained by this way (dendrites - crystals of α solid solution) have been determined, among others, by the angle of inclination with reference to the casting symmetry axis.

Simulation studies carried out with the help of Calcosoft 2D system with CAFE module have been preceded by determining the conditions of the experiment (geometric, physical, initial and boundary conditions) and by definition of variation range of selected parameters describing physical conditions of the experiment.
The simulation calculation has been performed for the following physical parameters:

**the parameters of constant values:**
- characteristic temperatures determined on the grounds of experimental curves of casting cooling: initial alloy temperature in the mould $660^\circ C$, liquidus $T_L = 602^\circ C$, eutectic $T_e = 574^\circ C$, solidus $T_S = 572.5^\circ C$, the mould and external $25^\circ C$;
- solidification heat of the alloy $419 \, 000 \, J/kg$;
- heat capacity, $kJ/(m^3 \cdot K)$: of the alloy in liquid phase $C'_L=3483$, in solid phase $C_S=1700$; of silica sand $C_{Kw}=1500$, insulating material (microsphere) $C_M=587$; chill $C_{Och}=3764$;
- heat-transfer coefficient, $W/(m^2 \cdot K)$: casting-mould $\alpha_{od.Kw}=10000$, $\alpha_{external}=20$;
- thermal conductivity, $W/(m \cdot K)$ of liquid $\lambda_L=90$ and solid phase $\lambda_S=130$;

**the parameters of varying values:**
- thermal conductivity of mould sand, $W/(m \cdot K)$: silica $\lambda_{Kw}=0.25-8$, insulating material (microsphere) $\lambda_M=0.1-0.6$;
- heat-transfer coefficient, $W/(m^2 \cdot K)$: casting-chill $\alpha_{od.Och}=200-2000$;
- maximal number of nuclei (grmax.gauss): a homogenous mould of silica sand: $n_v$ (in the bulk of liquid)=$10^3-10^{11} \, m^3$, $n_s$ (at the mould surface)=$10^6-10^{10} \, m^2$, a mould with a chill: $n_v=10^3-10^{11} \, m^3$, $n_s$ (at the mould surface)=$10^6-10^{10} \, m^2$, $n_{Och}$ (at the chill surface)=$10^8-10^{10} \, m^2$;
- undercooling (deltatm.gauss), K a homogenous mould: $\Delta T_v=1-4$, $\Delta T_s=1-10$, a mould with a chill: $\Delta T_v=1-15$, $\Delta T_s=1-30$, $\Delta T_{Och}$(at the chill)=1-30
- standard deviation (deltats.gauss), \( K \): a homogenous mould: \( \sigma_v \) (in the bulk of liquid)=0.14, \( \sigma_s \) (at the mould surface)=0.55, a mould with a chill: \( \sigma_v=0.01+15 \), \( \sigma_s=0.01+3 \), \( \sigma_{Och} \) (on the chill surface)=1+3.

Results of the simulation research have been analyzed with regard to geometric parameters of virtual structure (the shape, size, and location) obtained from the computation. Fig. 4, presents a comparison for the case of the best conformity with the experimental structure.

Such a comparison of geometric parameters of a virtual structure and experimental results indicates that the virtual structure simulated in the conditions approximating the situation occurring in a homogenous silica sand mould (Fig. 4a) remarkably differs from a real structure. A virtual structure simulated in the conditions approaching a mould of insulating material (microsphere) sand with a chill (more intensive heat transfer towards the chill D) distinguished with considerably different crystal sizes across the casting cross section. Approximation of inclination angle of dendritic crystals was satisfying, and, in some cases even good (Fig. 4b). In considered structures the nucleation
distribution (Fig. 5) at the surface of the mould, chill, and bulk of liquid was determined from \textit{à priori} assumed curves \(dn/d(\Delta T)=f(\Delta T)\) based on undercooling values calculated during the simulation (in accordance with the model of temperature difference between liquidus and growing dendrite tip temperature).

The data for purposes of calculation of a virtual structure have been acquired from the analysis of experimental results, with special attention paid to the relationship between undercooling level and dendritic structure resulting from metallographic studies. The values of undercooling at the casting cross section are shown in Fig. 6. Under solidification conditions corresponding to the sand mould (Fig. 6a) the points of minimal undercooling values are located in the distance 4÷6 mm from the symmetry axis of the cylindrical casting. Figure 6b presents the changeability of undercooling level in a solidifying casting under the conditions corresponding to the insulating (microsphere) mould with a chill, from the bottom of the casting surface.

Kinetics of crystal growth as a function of undercooling, determined on the grounds of the relationship \(\nu(\Delta T)=a_2\Delta T^2+a_3\,\Delta T^3\), is shown in Fig. 7. Values of the coefficients \(a_2=2,9\times10^6\) ms\(^{-1}\)K\(^{-2}\) and \(a_3=1,49\times10^6\) ms\(^{-1}\)K\(^{-3}\) are assumed from literature [3].
Fig. 6. Relationship of undercooling $\Delta T$ as a function of cylinder casting axis distance $X$ in various distances $y$ from the bottom surface of a cylinder casting: a) conditions for sand mould, b) conditions for mould with chill

Rys. 6. Zależność przechłodzenia $\Delta T$ w funkcji odległości x od osi walca w różnych odległościach y od dolnej powierzchni odlewu walcowego: a) warunki formy jednolitej, b) warunki formy z ochładzalnikiem

Fig. 7. Kinetics of the growth of Al-Si 7% alloy crystals as a function of local undercooling

Rys. 7. Prędkość wzrostu kryształów stopu Al-Si 7% w funkcji lokalnego przechłodzenia
4. CONCLUSIONS

The research work allows to formulate the following preliminary conclusions, related to feasibility of microstructure forecasting with the help of the Calcosoft CAFE-2D system. The system formally enables quantitative forecasting of a simplified structure of a solidifying casting, in the virtual sense, taking into account different grain sizes and their location. Such a prognosis consists in geometric image of the structure for the case of a single–phase (solid) solution. The alloys, in which the phase of solid solution (here the α-phase of hypoeutectic Al–Si alloy), must be considered with particular precautions.

The work states that values of the parameters describing thermal solidification conditions and hypothetic curves defining a priori the course of nucleation, affect the forecasted results of geometric parameters of the structure. This is confirmation of the fact that the CS CAFE model is sensitive to appropriately expressed obvious physical interactions leading to the transformations in the alloy structure. Nevertheless, it is sure that further investigation aimed at validation of the model is necessary, in accordance with the principles provided, among others, in our works [6,7,8].

REFERENCES

STRESZCZENIE

W pracy przedstawiono opis modelowania metodą Cellular Automaton - Finite Element oraz jego testowanie, połączone z próbą walidacji systemu Calcosoft (CS-CAFE). Podano wyniki identyfikacji wybranych parametrów; użytych w modelach stochastycznym i cieplnym wraz z określeniem ich wpływu na wyniki prognozowania geometrycznych parametrów mikrostruktury podeutektycznego stopu Al-Si. Walidacja została przeprowadzona metodą symulacyjno-eksperymentalną w zróżnicowanych warunkach cieplnych oddziaływania formy odlewniczej. Wykorzystano wyniki metalograficznych badań struktur specjalnie wykonanych odlewów.

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