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ESTIMATION OF NUCLEI DENSITY IN SOLIDIFYING CASTING USING THE KOLMOGOROV THEORY

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SUMMARY

In the paper the solidification process in the micro-macro scale is analyzed. The mathematical model of heat transfer in the domain considered bases on the Mehl-Johnson-Avrami-Kolmogorov theory. The capacity of internal heat source resulting from the latent heat evolution is, among others, the function of nuclei density. This parameter is estimated using the methods of inverse problem solution. The additional information necessary in order to identify the unknown parameter results from the cooling curves at the selected points from casting domain. On the stage of numerical algorithm construction the least squares criterion containing the sensitivity coefficients is applied. The solution has been obtained using the boundary element method.

Key words: crystallization process, inverse problems, parameter estimation method

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1. FORMULATION OF THE PROBLEM

Let us consider the solidification process in domain of pure metal (e.g. aluminium) which in equilibrium conditions solidifies at constant temperature T^* (solidification point). Transient temperature field in the domain considered describes the following equation

$$x \in \Omega: \; c\frac{\partial T(x,t)}{\partial t} = \lambda \nabla^2 T(x,t) + Q(x,t) \tag{1}$$

where c is the specific heat per unit of volume, λ is the thermal conductivity, $Q(x, t)$ is the source function, T, x, t denote temperature, spatial co-ordinates and time. Here the constant values of thermophysical parameters c and λ are assumed. It should be pointed out that the crystallization process proceeds in the rather small interval of temperature and this assumption does not introduce the essential errors.
The last component in equation (1) is equal to

$$Q(x,t) = L\frac{\partial f_S(x,t)}{\partial t} \tag{2}$$

where $f_S(x, t)$ is the solid state fraction in the region of the point considered, while L is the latent heat per unit of volume.

A temporary value of solid state fraction of the metal at the point from casting domain is given by the Mehl-Johnson-Avrami-Kolmogorov type equation [1, 2]

$$f_S(x,t) = 1 - \exp\left[-\frac{4}{3}\pi N\left(\int_0^t u(x,\tau)\,\mathrm{d}\tau\right)^3\right] \tag{3}$$

where N is a constant number of nuclei (more precisely: density [nuclei/m^3]), $u(x, t)$ is the rate of solid phase growth.
The solid phase growth (equiaxial grains) is determined by following formula

$$u(x,t) = \frac{\partial R(x,t)}{\partial t} = \mu \Delta T^2(x,t) \tag{4}$$

where R is a grain radius, μ is the growth coefficient, and $\Delta T(x,t) = T^* - T(x,t)$ is the undercooling below a solidification point. Taking into account the formulas (2), (3), (4), the source function in equation (1) can be written as follows

$$Q(x,t) = 4\pi N L \mu \Delta T^2(x,t) r^2 \exp\left(-\frac{4}{3}\pi N r^3\right) \tag{5}$$

where

$$r = r(x,t) = \int_0^t \mu \Delta T^2(x,\tau)\,\mathrm{d}\tau \tag{6}$$

The equation (1) is supplemented by the boundary condition

$$x \in \Gamma: \quad T(x,t) = T_b \tag{7}$$

where T_b is the known boundary temperature resulting from the Schwarz solution [3]. The initial condition is also given, namely

$$t = 0: \quad T(x,0) = T_p \tag{8}$$

where T_p is the pouring temperature.

For direct problem the boundary and initial conditions as well as the parameters appearing in the mathematical model are known and we determine the temperature distribution $T(x, t)$. For the inverse problem analyzed we assume that the nuclei density N is unknown. In order to identify the parameter N the additional information is necessary. So, we assume that the values of temperature T_{di}^f at the selected set of points x_i (sensors) from casting domain for times t^f are known, namely

$$T_{di}^f = T_d\left(x_i, t^f\right), \quad i = 1,2,...,M, \quad f = 1,2,...,F \tag{9}$$

2. METHOD OF SOLUTION

In order to solve the inverse problem, the least squares criterion is applied [4]

$$S(N) = \sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f - T_{di}^f\right)^2 \tag{10}$$

where $T_i^f = T(x_i, t^f)$ is the calculated temperature at the point x_i for time t^f. Differentiating the criterion (10) with respect to the unknown nuclei density and using the necessary condition of minimum, one obtains

$$\frac{\partial S}{\partial N} = 2\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f - T_{di}^f\right)\frac{\partial T_i^f}{\partial N}\bigg|_{N=N^k} = 0 \tag{11}$$

where k is the number of iteration, N^k for k =0 is the arbitrary assumed value of N, while N^k for $k > 0$ results from the previous iteration.
Function T_i^f is expanded in a Taylor series about known value of N^k, this means

$$T_i^f = \left(T_i^f\right)^k + \left(U_i^f\right)^k \left(N^{k+1} - N^k\right) \tag{12}$$

where

$$\left(U_i^f\right)^k = \left.\frac{\partial T_i^f}{\partial N}\right|_{N=N^k} \tag{13}$$

are the sensitivity coefficients. Putting (12) into (11), after the simple mathematical manipulations, one has

$$N^{k+1} = N^k \frac{\sum_{i=1}^{M}\sum_{f=1}^{F}\left(U_i^f\right)^k \left[T_{di}^f - \left(T_i^f\right)^k\right]}{\sum_{i=1}^{M}\sum_{f=1}^{F}\left[\left(U_i^f\right)\right]^2}, \quad k = 0,1,...,K \tag{14}$$

This equation allows to find the values of N^{k+1}. The iteration process is stopped when the assumed accuracy is achieved.

In order to determine the sensitivity coefficients (13), the equations (1), (7), (8) are differentiated with respect to N and then

$$\begin{cases} x \in \Omega: & c\dfrac{\partial U(x,t)}{\partial t} = \lambda \nabla^2 U(x,t) + Q_U(x,t) \\ x \in \Gamma: & U(x,t) = 0 \\ t = 0: & U(x,t) = 0 \end{cases} \tag{15}$$

where $U(x,t) = \partial T(x,t)/\partial N$, $Q_U(x,t) = \partial Q(x,t)/\partial N$ and the function Q_U (x, t) is following

$$\begin{gathered} Q_U(x,t) = 4\pi\mu L \exp\left(-\frac{4}{3}\pi N r^3\right) r \cdot \\ \left\{\Delta T^2(x,t)\left[r - \frac{4}{3}\pi N r^4 + 4\pi N^2 r^3 r_U - 2N r_U\right] - 2N\Delta T(x,t) U(x,t) r\right\} \end{gathered} \tag{16}$$

where

$$r_U = r_U(x,t) = \int_0^t \mu \Delta T(x,\tau) U(x,t)\,\mathrm{d}\tau \tag{17}$$

For each iteration the basic problem and additional one connected with the sensitivity function have been solved using the 1st scheme of the boundary element method [2, 3].

3. RESULTS OF COMPUTATIONS

As an example, the 1D problem has been solved. The plate of thickness $L = 0.03$ [m] made from aluminum has been considered. The following input data are assumed: thermal conductivity $\lambda = 150$ [W/(mK)], volumetric specific heat $c = 2.875 \cdot 10^6$ [J/(m^3 K)], latent heat per unit of volume $L = 9.75 \cdot 10^8$ [J/m^3], solidification point $T^* = 660$ °C, growth coefficient $\mu = 3 \cdot 10^{16}$ [m/K^{2}s], initial temperature $T_p = 662$ °C, boundary temperature $T_b = 650$ °C.

In order to estimate the value of N the courses of cooling curves (c.f. equation (9)) at the points 1 - 0.0015 [m] (distance between the point and the boundary of plate), 2 - 0.0035 [m] and 3 - 0.0055 [m] have been taken into account - Figure 1. They result from the direct problem solution under the assumption that $N = 10^{10}$ [nuclei/m^3].

Figure 2 illustrates the solution of inverse problem for different initial values of N^0. It is visible that the iteration process is convergent and the solution close to the exact value is obtained after the several iterations.

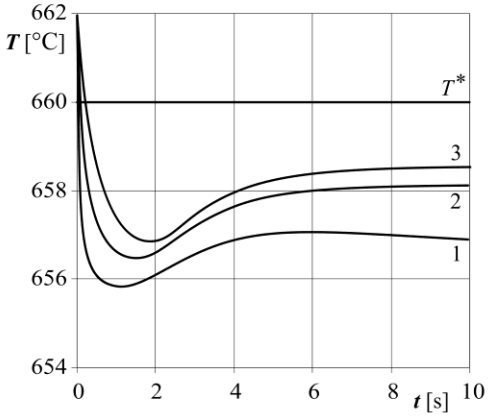

Fig. 1. Cooling curves
Rys. 1. Krzywe stygnięcia

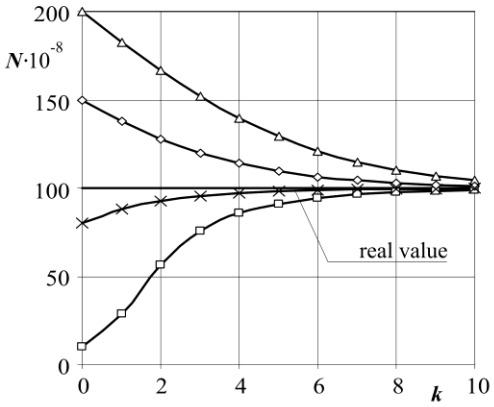

Fig. 2. Inverse problem solution
Rys. 2. Rozwiązanie zadania odwrotnego

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OSZACOWANIE GĘSTOŚCI ZARODKÓW W KRZEPNĄCYM ODLEWIE Z WYKORZYSTANIEM TEORII KOŁMOGOROWA

STRESZCZENIE

W artykule analizowano proces krzepnięcia w skali mikro-makro. Model matematyczny przepływu ciepła w obszarze bazuje na teorii Mehla-Johnsona-Avrami-Kołmogorowa. Wydajność wewnętrznych źródeł ciepła związana z wydzielaniem się ciepła krzepnięcia jest zależna między innymi od gęstości zarodków. Oszacowanie tego parametru uzyskano rozwiązując zadanie odwrotne, w którym wykorzystano dodatkową informację dotyczącą przebiegu krzywych stygnięcia w kilku punktach odlewu. Algorytm bazuje na kryterium najmniejszych kwadratów, w którym występują tzw. współczynniki wrażliwości.

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