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# MODELLING OF PURE METAL CRYSTALLIZATION PROCESS WITH REGARD TO SENSITIVITY ANALYSIS

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SUMMARY

In the paper the sensitivity analysis of pure metal crystallization process with respect to the number of nuclei $N$ and growth coefficient $\mu$ is presented. The basic problem and additional problems connected with the sensitivity analysis are solved using the boundary element method. In the final part the results of computations are shown.

*Key words: crystallization, numerical modelling, sensitivity analysis*

## 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 domain considered describes the following equation

$$x \in \Omega: \quad c(T)\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] + Q(x,t) \tag{1}$$

where $c(T)$ is the specific heat per unit of volume, $\lambda(T)$ is the thermal conductivity,

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$Q(x,t)$ is the source function, *T, x, t* denote temperature, spatial coordinates and time. The last component in equation (1) is equal to

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

where $f_S(x,t)$ is the solid state fraction in the region of the point considered, while $L_V$ is the latent heat per unit of volume.
A temporary value of solid state fraction of the metal at the point of casting domain is given by the Johnson – Mehl – 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, $\mu$ is the growth coefficient, and $\Delta T(x,t) = T^* - T(x,t)$ is the undercooling below a solidification point.
In order to simplify the further considerations we assume the constant values of thermophysical parameters $c$ and $\lambda$ (the crystallization process proceeds in the rather small interval of temperature and this assumption does not introduce the essential errors). So, the equation (1) can be written in the form

$$c\frac{\partial T(x,t)}{\partial t} = \lambda \nabla^2 T(x,t) + Q(x,t) \tag{5}$$

where (c.f. formulas (2), (3), (4) )

$$Q(x,t) = 4\pi N L_V \mu \Delta^2 T(x,t) r^2 \exp\left( -\frac{4}{3}\pi N r^3 \right) \tag{6}$$

while

$$r = r(x,t) = \int_0^t \mu \Delta^2 T(x,\tau) \mathrm{d}\tau \tag{7}$$

The equation (5) is supplemented by the boundary condition

$$x \in \Gamma: \quad T(x,t) = T_b \tag{8}$$

where $T_b$ is the known boundary temperature resulting from the Schwarz solution [4]. The initial condition is also given, namely

$$t = 0: \quad T(x,0) = T_p \tag{9}$$

where $T_p$ is the pouring temperature.

## 2. SENSITIVITY ANALYSIS WITH RESPECT TO μ AND N

In this paper the sensitivity analysis of temperature field in domain of solidification casting with respect to the crystallization parameters, namely the growth coefficient μ and number of nuclei $N$ is done.

At first, the equations (5), (8), (9) are differentiated with respect to μ and then one obtains

$$\begin{cases} x \in \Omega: \quad c\dfrac{\partial U(x,t)}{\partial t} = \lambda \nabla^2 U(x,t) + Q_U(x,t) \\ x \in \Gamma: \quad U(x,t) = 0 \\ t = 0: \quad U(x,t) = 0 \end{cases} \tag{10}$$

where $U(x,t) = \partial T(x,t)/\partial\mu$, $Q_U(x,t) = \partial Q(x,t)/\partial\mu$. The function $Q_U(x,t)$ equals

$$\begin{aligned} Q_U(x,t) = 4\pi N L_V \exp\left(-\frac{4}{3}\pi N r^3\right) r \Big\{ \Delta^2 T(x,t) \cdot \\ \left[3r - 4\pi N r^4 + 8\pi N \mu r^3 r_U - 4\mu r_U\right] - 2\mu \Delta T(x,t) U(x,t) r \Big\} \end{aligned} \tag{11}$$

where

$$r_U = r_U(x,t) = \int_0^t \mu \Delta T(x,\tau)\, U(x,\tau) \mathrm{d}\tau \tag{12}$$

In similar way, the equations (5), (8), (9) are differentiated with respect to $N$ and then

$$\begin{cases} x \in \Omega: \quad c\dfrac{\partial W(x,t)}{\partial t} = \lambda \nabla^2 W(x,t) + W_U(x,t) \\ x \in \Gamma: \quad W(x,t) = 0 \\ t = 0: \quad W(x,t) = 0 \end{cases} \tag{13}$$

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

$$\begin{aligned} Q_W(x,t) = 4\pi\mu L_V \exp\left(-\frac{4}{3}\pi N r^3\right) r \Big\{ \Delta^2 T(x,t) \cdot \\ \left[ r - \frac{4}{3}\pi N r^4 + 8\pi N^2 r^3 r_W - 4 N r_W \right] - 2 N \Delta T(x,t) W(x,t) r \Big\} \end{aligned} \tag{14}$$

where

$$r_W = r_W(x,t) = \int_0^t \mu \Delta T(x,\tau)\, W(x,\tau)\, \mathrm{d}\tau \tag{15}$$

The additional problems connected with the functions $U(x,t)$ and $W(x,t)$ are coupled with the basic one by source functions $Q_U(x,t)$ and $Q_W(x,t)$ in which the value $\Delta T(x,t)$ appears.

## 3. SOLUTION OF THE PROBLEM AND RESULTS OF COMPUTATIONS

In order to solve the basic problem and additional ones connected with the sensitivity analysis, the boundary element method has been used. At first, the time grid with constant step $\Delta t = t^f - t^{f-1}$ is introduced. The 1st scheme of the BEM for each transition $t^{f-1} \to t^f$ requires the solution of three adequate systems of equations connected with boundary values of functions $T(x,t^f)$, $U(x,t^f)$, $W(x,t^f)$ and boundary values of fluxes, this means $q(x,t^f) = -\lambda \partial T(x,t^f)/\partial n$, $q_U(x,t^f) = -\lambda \partial U(x,t^f)/\partial n$, $q_W(x,t^f) = -\lambda \partial W(x,t^f)/\partial n$. The knowledge of these boundary values allows to determine the temperature $T(x,t^f)$ and functions $U(x,t^f)$, $W(x,t^f)$ at the internal points of the domain considered. The details concerning the BEM algorithm can be found among others in [3].

In the paper the 1D problem has been solved. The plate of thickness $L$=0.01 [m] made from aluminium has been considered. The following input data are assumed: thermal

conductivity λ=150 [W/mK], volumetric specific heat $c$=2.5·10$^7$ [J/Km$^3$], latent heat per unit of volume $L_V$ =9.75·10$^8$ [J/m$^3$], solidification point $T^*$=660 [K], number of nuclei $N$=10$^{10}$ [1/m$^3$], growth coefficient μ=3·10$^{-6}$ [m/sK$^2$], initial temperature $T_p$=680 [K], boundary temperature $T_b$=655 [K].

Figure 1 illustrates the courses of source functions $Q(x_i,t)$ at selected points of casting, while Figures 2 and 3 show the courses of functions $Q_U(x_i,t)$ and $Q_W(x_i,t)$ at the same points. The distances between these points and the boundary of casting are following 1 – 4.5 [mm], 2 – 3.5 [mm], 3 – 2.5 [mm], 4 – 1.5 [mm], 5 – 0.5 [mm].

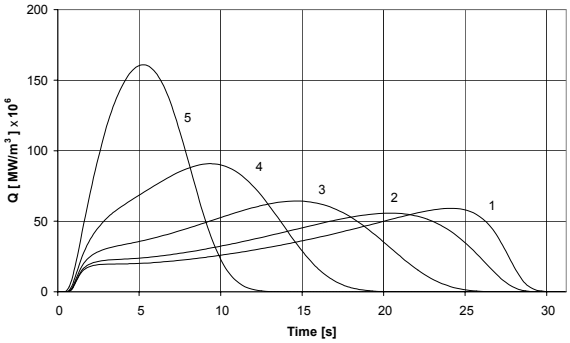


Fig. 1. Source functions $Q(x_i,t)$

Rys. 1. Funkcje źródła $Q(x_i,t)$

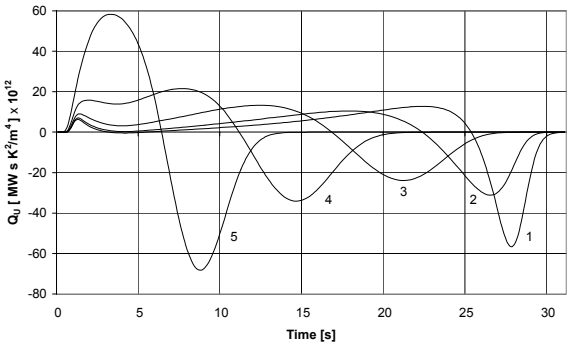


Fig. 2. Course of functions $Q_U(x_i,t)$

Rys. 2. Przebieg funkcji $Q_U(x_i,t)$

Sensitivity analysis allows to estimate the changes of temperature due to the changes of parameters μ and $N$, namely

$$\Delta T_{\mu}(x,t) = T(\mu + \Delta\mu, N, x, t) - T(\mu - \Delta\mu, N, x, t) = 2U(x,t)\Delta\mu \tag{16}$$

and

$$\Delta T_{N}(x,t) = T(\mu, N + \Delta N, x, t) - T(\mu, N - \Delta N, x, t) = 2W(x,t)\Delta N \tag{17}$$

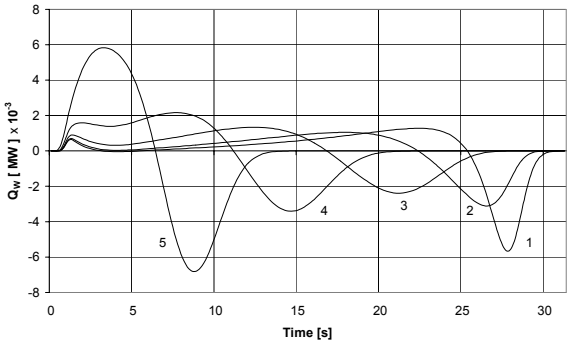


Fig. 3. Course of functions $Q_W(x_i,t)$

Rys. 3. Przebieg funkcji $Q_W(x_i,t)$

For the assumed value $\Delta\mu=0.5\cdot10^{-6}$ the maximum change of temperature $\Delta T_{\mu\,\max}(x, t)$= 1.7 [ $^0$C] has been obtained. For value $\Delta N=0.5\cdot10^{10}$ the maximum change of temperature is equal to $\Delta T_{N\,\max}(x, t)$= 1.8 [ $^0$C].

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## MODELOWANIE PROCESU KRYSTALIZACJI CZYSTEGO METALU Z UWZGLĘDNIENIEM ANALIZY WRAŻLIWOŚCI

STRESZCZENIE

W pracy przedstawiono analizę wrażliwości procesu krystalizacji czystego metalu ze względu na liczbę ziaren $N$ i współczynnik wzrostu $\mu$. Zadanie podstawowe i problemy dodatkowe wynikające z analizy wrażliwości rozwiązano stosując metodę elementów brzegowych. W końcowej części artykułu przedstawiono wyniki obliczeń.

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