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Modelling of crystallization process using the interval boundary element method

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The mathematical model of solidification process can be formulated using the macro or micro-macro approach. In this paper the second generation model (micro-macro one) is considered. The driving force of crystallization is the local and temporary undercooling below solidification point T_{cr}. The nucleation and nuclei growth are proportional to the second power of undercooling. Formulas determining the phenomena previously mentioned contain coefficients called the nucleation coefficient and nuclei growth one. These coefficients are assumed to be interval values. For above assumptions the problem has been solved by means of interval boundary element method. In the final part of the paper the results of computations are shown.

Keywords: interval boundary element method, interval arithmetic, crystallization

1. Introduction

The solidification process proceeding in the volume of pure metal or alloy can be treated as a macroscopic one [7], but a more exact approach requires to regard the microscopic aspects of the phenomena considered, in particular the nucleation and nuclei growth [3–5]. The Fourier-Kirchhoff equation (energy equation) determining the course of thermal processes in the system considered contains the term controlling the kinetics of solidification (source function). This term is proportional to the solidification rate (more precisely, to the time derivative of local volumetric solid state fraction S). The changes of S are determined by the changes of nuclei density and temporary grains dimensions. In the paper the exponential model of crystallization proposed by Mehl–Johnson–Avrami–Kolmogoroff is applied [3, 5]. Such approach is widely known, but the parameters appearing in the crystallization model this means nucleation coefficient and nuclei growth coefficient are, as a rule, treated as the constant values, while in the model here presented nucleation and growth coefficients are assumed to be interval values (as an example the paper [2] can be quoted). In order to solve the problem formulated the interval boundary element method for transient heat diffusion has been applied [9]. The examples of computations confirm the efficiency of proposed approach for solidification process modelling.

2. Model of crystallization

Let us consider the solidification process in domain of pure metal (e.g. aluminium) which in equilibrium conditions solidifies at the constant temperature T_{cr} (solidification point). Transient temperature field in domain Ω describes the following energy equation,

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

where c is the volumetric specific heat, λ is the thermal conductivity, $Q(x,t)$ is the source function, T, x, t denote temperature, spatial co-ordinates and time, respectively.

The source function $Q(x,t)$ can be expressed as follows,

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

where L is the volumetric latent heat, $S(x,t)$ is the volumetric fraction of the solid state at the neighborhood of the point considered x.

The typical feature of the models for which the micro processes are taken into account, is an analysis of $S(x,t)$ on the basis of crystallization processes theory. For instance, the following function can be introduced [5],

$$\omega(x,t) = N(x,t)V(x,t), \tag{3}$$

where $N(x,t)$ is a grains density [grains/m^3], $V(x,t)$ is a single grain volume. If we consider the spherical grains then denoting by $R(x,t)$ a temporary radius of single grain one has

$$\omega(x,t) = \frac{4}{3}\pi N(x,t)R(x,t)^3. \tag{4}$$

In this paper the exponential solidification model proposed by Mehl–Johnson–Avrami–Kolmogoroff is applied and then

$$S(x,t) = 1 - \exp[-\omega(x,t)] \tag{5}$$

or

$$S(x,t) = 1 - \exp\left[-\frac{4}{3}\pi\, N(x,t)\, R(x,t)^3\right]. \tag{6}$$

Denoting by $u(x,t)$ the solidification rate, this means

$$u(x,t) = \frac{\partial R(x,t)}{\partial t}, \tag{7}$$

we have

$$R(x,t) = \int_0^t u(x,\tau)\,\mathrm{d}\tau. \tag{8}$$

The time derivative of function $S(x,t)$ is calculated and finally the function $Q(x,t)$ (c.f. Eq. (2)) takes the form

$$Q(x,t) = \frac{4}{3}\pi L\left[\frac{\partial N(x,t)}{\partial t}\, R(x,t)^3 + 3N(x,t)\, R(x,t)^2 u(x,t)\right] \exp\left[-\frac{4}{3}\pi\, N(x,t)\, R(x,t)^3\right]. \tag{9}$$

Additionally, the undercooling below the solidification point T_{cr} is defined as follows,

$$\Delta T(x,t) = \begin{cases} T_{cr} - T(x,t), & T(x,t) \le T_{cr}, \\ 0, & T(x,t) > T_{cr}. \end{cases} \tag{10}$$

It is assumed that the local and temporary number of nuclei is proportional to the second power of undercooling

$$N(x,t) = \gamma \Delta T(x,t)^2 \tag{11}$$

where γ is the nucleation coefficient. The nucleation stops at maximum undercooling.

The solidification rate is determined by the formula

$$u(x,t) = \mu \Delta T(x,t)^2 \tag{12}$$

where μ is the growth coefficient.

The mathematical description of the problem is supplemented by adequate boundary and initial conditions.

The solution of the boundary-initial problem discussed requires knowledge of coefficients γ and μ. Experimental estimations of these values are difficult because they are dependent (among others) on technological conditions, object geometry etc. So, it seems that both γ and μ should be treated as interval values and this assumption is closer to the real physical conditions of the process.

3. Interval source function

Let us consider the interval values of the nucleation coefficient $\tilde{\gamma} = \langle \underline{\gamma}, \bar{\gamma} \rangle$ and the growth coefficient $\tilde{\mu} = \langle \underline{\mu}, \bar{\mu} \rangle$ [8]. By this way the grain density $\tilde{N}(x,t)$ and the solidification rate $\tilde{u}(x,t)$ are interval values

$$\tilde{N}(x,t) = \tilde{\gamma} \Delta T(x,t)^2 \tag{13}$$

and

$$\tilde{u}(x,t) = \tilde{\mu} \Delta T(x,t)^2 \tag{14}$$

where the undercooling can be defined as follows,

$$\Delta T(x,t) = \begin{cases} T_{cr} - \frac{1}{2}\left[\underline{T}(x,t) + \bar{T}(x,t)\right], & \frac{1}{2}\left[\underline{T}(x,t) + \bar{T}(x,t)\right] \leq T_{cr}, \\ 0, & \frac{1}{2}\left[\underline{T}(x,t) + \bar{T}(x,t)\right] > T_{cr}, \end{cases} \tag{15}$$

while $\underline{T}(x,t)$ and $\bar{T}(x,t)$ denote the first and the second endpoints of the temperature interval, respectively.

The temporary interval radius of the single grain is defined as (c.f. Eq. (8))

$$\tilde{R}(x,t) = \int_0^t \tilde{\mu} \Delta T(x,\tau)^2 \, \mathrm{d}\tau \tag{16}$$

and then the interval source function can be expressed as follows,

$$\tilde{Q}(x,t) = \frac{4}{3}\pi L \left[\frac{\partial \tilde{N}(x,t)}{\partial t} \tilde{R}(x,t)^3 + 3\tilde{N}(x,t)\, \tilde{R}(x,t)^2 \tilde{u}(x,t) \right] \exp\left[-\frac{4}{3}\pi \tilde{N}(x,t)\, \tilde{R}(x,t)^3 \right]. \tag{17}$$

This interval function has to be calculated according to the rules of the interval arithmetic [7].

4. Interval boundary element method

At first the time grid is introduced,

$$0 = t^0 < t^1 < t^2 < \cdots < t^{f-1} < t^f < \cdots < t^F < \infty, \tag{18}$$

with a constant time step $\Delta t = t^f - t^{f-1}$.

If the first scheme of the BEM is taken into account [1, 6, 9] then the boundary integral equation corresponding to the transition $t^{f-1} \to t^f$ is of the form

$$B(\xi)\,T(\xi,t^f) + \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\int_{\Gamma} T^*(\xi,x,t^f,t)\,q(x,t^f)\,\mathrm{d}\Gamma\mathrm{d}t$$

$$= \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\int_{\Gamma} q^*(\xi,x,t^f,t)\,T(x,t^f)\,\mathrm{d}\Gamma\mathrm{d}t + \iint_{\Omega} T^*(\xi,x,t^f,t^{f-1})\,T(x,t^{f-1})\,\mathrm{d}\Omega$$

$$+ \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\iint_{\Omega} Q(x,t)\,T^*(\xi,x,t^f,t^{f-1})\,\mathrm{d}\Omega\mathrm{d}t \tag{19}$$

where ξ is the observation point, $B(\xi)$ is the coefficient from the interval $(0,1)$. The fundamental solution $T^*(\xi,x,t^f,t)$ [1, 6, 9] is defined as follows,

$$T^*(\xi,x,t^f,t) = \frac{1}{4\pi a(t^f-t)}\exp\left[-\frac{r^2}{4a(t^f-t)}\right], \tag{20}$$

where $a = \lambda/c\rho$, r is the distance from the point under consideration x to the observation point ξ, while

$$q^*(\xi,x,t^f,t) = -\lambda\frac{\partial T^*(\xi,x,t^f,t)}{\partial n} \tag{21}$$

and

$$q(x,t) = -\lambda\frac{\partial T(x,t)}{\partial n}\,. \tag{22}$$

In case of an interval source function the boundary integral equation has the following form,

$$B(\xi)\,\tilde{T}(\xi,t^f) + \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\int_{\Gamma} T^*(\xi,x,t^f,t)\,\tilde{q}(x,t^f)\,\mathrm{d}\Gamma\mathrm{d}t$$

$$= \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\int_{\Gamma} q^*(\xi,x,t^f,t)\,\tilde{T}(x,t^f)\,\mathrm{d}\Gamma\mathrm{d}t + \iint_{\Omega} T^*(\xi,x,t^f,t^{f-1})\,\tilde{T}(x,t^{f-1})\,\mathrm{d}\Omega$$

$$+ \frac{1}{c\rho}\int_{t^{f-1}}^{t^f}\iint_{\Omega} \tilde{Q}(x,t)\,T^*(\xi,x,t^f,t^{f-1})\,\mathrm{d}\Omega\mathrm{d}t, \tag{23}$$

If we use constant elements with respect to time then Eq. (23) takes a form

$$B(\xi)\,\tilde{T}(\xi,t^f) + \int_{\Gamma}\tilde{q}(x,t^f)\,g(\xi,x)\,\mathrm{d}\Gamma$$

$$= \int_{\Gamma}\tilde{T}(x,t^f)\,h(\xi,x)\,\mathrm{d}\Gamma + \iint_{\Omega} T^*(\xi,x,t^f,t^{f-1})\,\tilde{T}(x,t^{f-1})\,\mathrm{d}\Omega$$

$$+ \iint_{\Omega}\tilde{Q}(x,t^{f-1})\,g(\xi,x)\,\mathrm{d}\Omega \tag{24}$$

where

$$h(\xi, x) = \frac{1}{c\rho} \int_{t^{f-1}}^{t^f} q^*(\xi, x, t^f, t)\, \mathrm{d}t \tag{25}$$

and

$$g(\xi, x) = \frac{1}{c\rho} \int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\, \mathrm{d}t\,. \tag{26}$$

In numerical realization we consider the following discrete form of the interval equation (24) (for the constant boundary elements and constant internal cells),

$$\sum_{j=1}^{N} G_{ij}\tilde{q}_j^f = \sum_{j=1}^{N} H_{ij}\tilde{T}_j^f + \sum_{l=1}^{L} P_{il}\tilde{T}_l^{f-1} + \sum_{l=1}^{L} Z_{il}\tilde{Q}_l^{f-1}, \tag{27}$$

where

$$G_{ij} = \int_{\Gamma_j} g(\xi^i, x)\, \mathrm{d}\Gamma_j\,, \tag{28}$$

$$H_{ij} = \begin{cases} \int_{\Gamma_j} h(\xi^i, x)\, \mathrm{d}\Gamma_j\,, & i \neq j, \\ -0.5, & i = j, \end{cases} \tag{29}$$

$$P_{il} = \iint_{\Omega_l} T^*(\xi, x, t^f, t^{f-1})\, \mathrm{d}\Omega_l\,, \tag{30}$$

$$\dot{Z}_{il} = \iint_{\Omega_l} g(\xi^i, x)\, \mathrm{d}\Omega_l\,. \tag{31}$$

The system of equations (27) can be written in the matrix form, namely

$$\mathbf{G} \cdot \tilde{\mathbf{q}}^f = \mathbf{H} \cdot \tilde{\mathbf{T}}^f + \mathbf{P} \cdot \tilde{\mathbf{T}}^{f-1} + \mathbf{Z} \cdot \tilde{\mathbf{Q}}^{f-1}\,. \tag{32}$$

After the determining the 'missing' boundary values of $\tilde{T}$ and $\tilde{q}$, the values of the temperature $\tilde{T}$ at the internal points ξ^i for time t^f can be calculated using the formula

$$\tilde{T}_i^f = \sum_{j=1}^{N} H_{ij}\tilde{T}_j^f - \sum_{j=1}^{N} G_{ij}\tilde{q}_j^f + \sum_{l=1}^{L} P_{il}\tilde{T}_l^{f-1} + \sum_{l=1}^{L} Z_{il}\tilde{Q}_l^{f-1}. \tag{33}$$

In the special situation when only the term determining capacity of internal heat sources is an interval value the matrix elements G_{ij}, H_{ij}, P_{il}, Z_{il} are constant. It causes that in such a case IBEM algorithm is essentially simpler in comparison with the variant corresponding to the interval thermophysical parameters λ, c, ρ [9]. On the other hand the interval calculations of function $\tilde{Q}$ connected with the crystallization process modelling require to take into account the interval nucleation and the nuclei growth.

5. EXAMPLE OF COMPUTATIONS

The crystallization process proceeding in an aluminium bar of square section ($0.02 \times 0.02\,[\mathrm{m}]$) has been analyzed. On the external boundary the Dirichlet condition $T_b = 650\,[^\circ\mathrm{C}]$ has been assumed. The symmetrical fragment of the domain considered has been taken into account. The boundary has been divided into 40 constant boundary elements, the interior has been divided into 100 constant internal cells — see Fig. 1.

The following input data have been introduced: initial temperature $T_0 = 670\,[^\circ\mathrm{C}]$, solidification point $T_{cr} = 660\,[^\circ\mathrm{C}]$, thermal conductivity $\lambda = 180\,[\mathrm{W/mK}]$, specific heat $c = 1200\,[\mathrm{J/kgK}]$, density $\rho = 2500\,[\mathrm{kg/m^3}]$, volumetric latent heat $L = 975\,[\mathrm{MJ/m^3}]$, nuclei coefficient $\tilde{\gamma} = \langle 10^9 - 1000\,,\, 10^9 + 1000\rangle\,[1/\mathrm{K^2m^3}]$, growth coefficient $\tilde{\mu} = \langle 2.95 \cdot 10^{-6}\,,\, 3.05 \cdot 10^{-6}\rangle\,[\mathrm{m/sK^2}]$, time step $\Delta t = 0.002\,[\mathrm{s}]$.

Figures 2 and 3 illustrate the cooling curves obtained at the nodes 83 and 107 of the domain considered, where T_L, T_R denote the lower and the upper bounds of the temperature intervals.

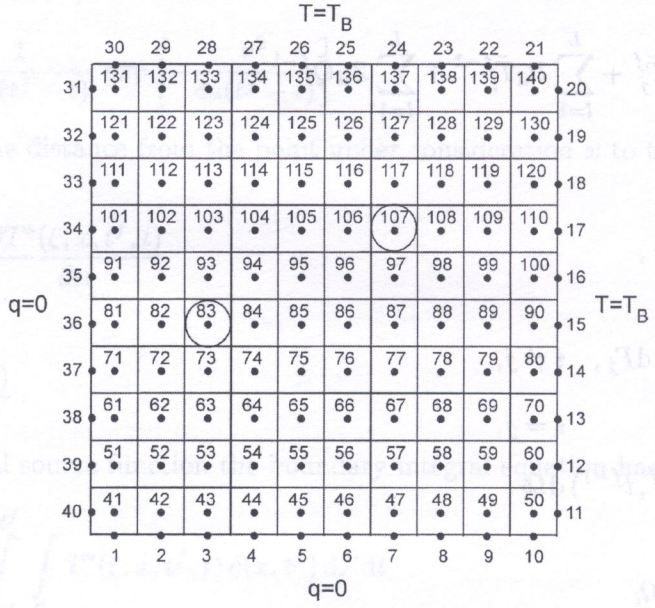

Fig. 1. Discretization of the domain Ω

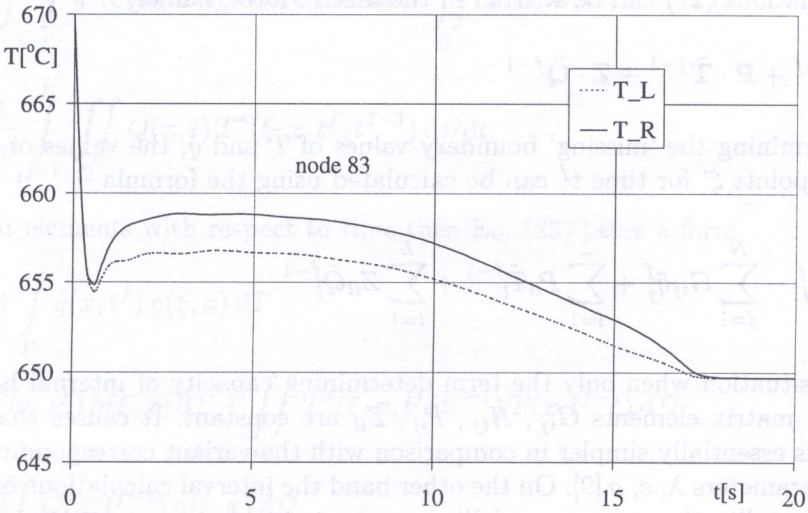

Fig. 2. Cooling curves at node 83

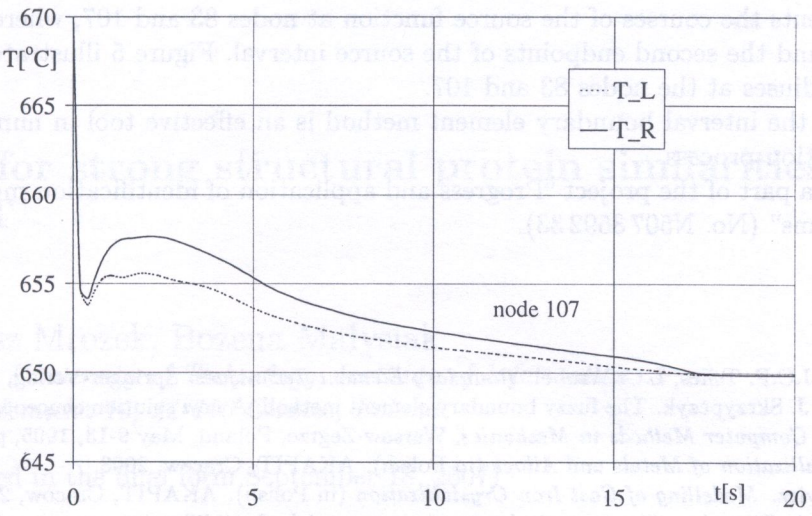

Fig. 3. Cooling curves at node 107

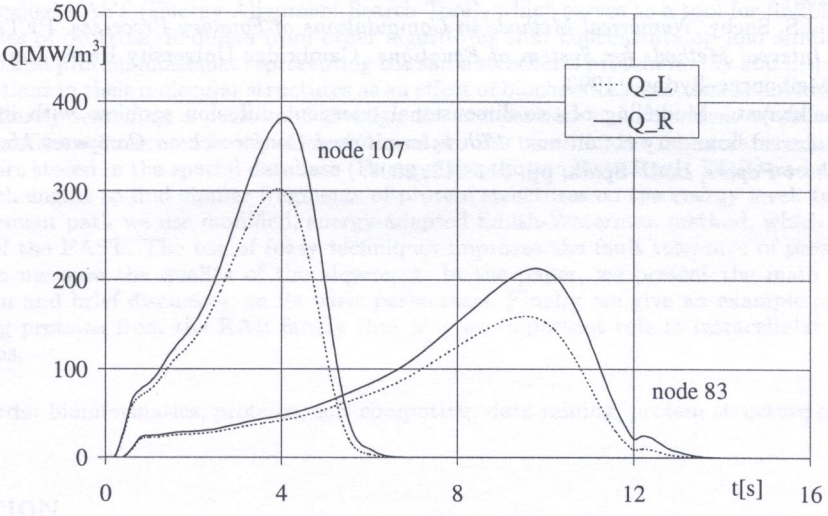

Fig. 4. The courses of the source function

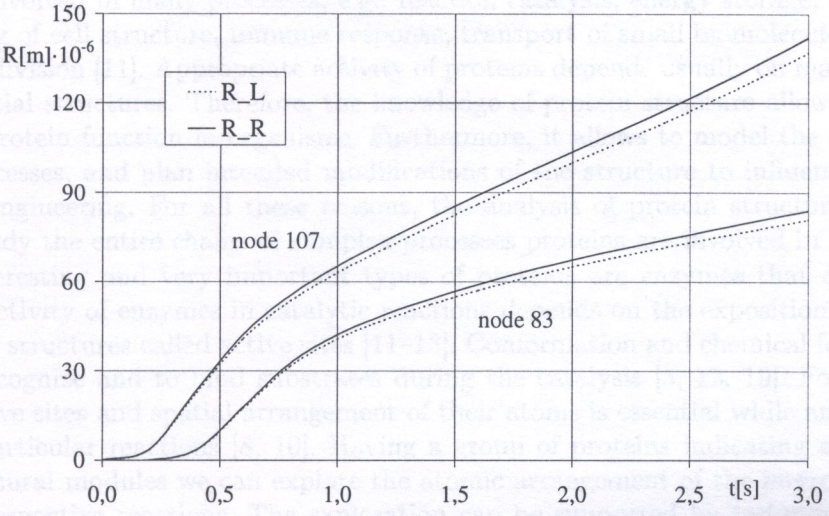

Fig. 5. The courses of the radius

Figure 4 presents the courses of the source function at nodes 83 and 107, where Q_L and Q_R denote the first and the second endpoints of the source interval. Figure 5 illustrates the temporary interval mean radiuses at the nodes 83 and 107.

Summing up, the interval boundary element method is an effective tool in numerical modelling of the crystallization process.

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