NUMERICAL MODEL OF SOLIDIFICATION OF CAST COMPOSITE WITH PARTICLES

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In the paper the numerical model of heat transfer in non-homogeneous domain (cast composite) is considered. The composite is formed by the spherical particles (Pb) and the metal matrix (Al). Initial temperatures of components correspond to solid state (particle) and liquid one (matrix). The heat is transferred from the aluminum matrix and absorbed by the lead particle. The 3D problem, i.e. the cubic control volume with single spherical particle located at the center part of the cube, is considered. A numerical algorithm corresponding to the discussed mathematical model of the boundary-initial problem is constructed on the basis of control volume method and some examples of numerical results are shown.

Keywords: cast composite, solidification, numerical modeling, control volume
method

1. INTRODUCTION

The macrostructure of the material considered is shown in Figure 1 [3]. In Figure 1b a single Pb particle with primary α phase crystals is presented. The non-homogeneous system created by the spherical particles (pure Pb) and matrix (pure Al) is being considered – Figure 2. The macro sub-domain analyzed is
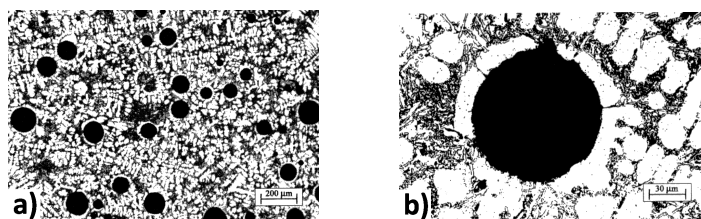

Fig. 1. a) The microstructure of AK9-Pb composite,
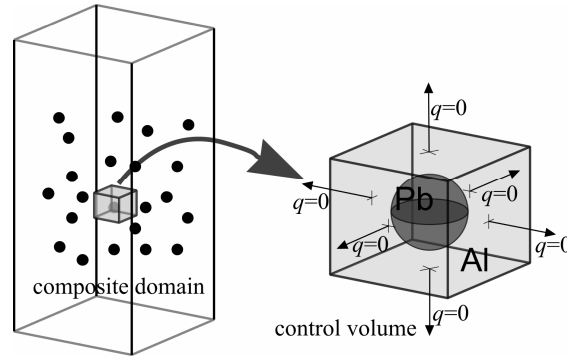b) Single Pb particle with primary α phase crystals

Fig. 2. The cast composite domain

located in the central part of the casting section. In this cube-shaped macro sub-domain the single spherical particle is located at the central part of the cube. This assumption allows us to neglect the influence of the boundary conditions given on the outer surface of the system. Hence, non-flux boundary conditions related to the sub-domain considered can be taken into account, i.e. in the interior of the casting domain the small temperature gradients are considered (volumetric solidification). The side of cube l results from the assumed diameter d and the volume fraction fr of the lead particle

$$l = d \cdot \sqrt[3]{\pi/(6 \cdot fr)} \qquad (1.1)$$

The initial temperature of aluminum matrix corresponds to the liquid state, while the initial temperature of lead particle corresponds to the solid one. The ideal thermal contact between the particle and the matrix is assumed. The solidifying matrix and the melting particle are located within the macro sub-domain analyzed with adiabatic walls. Thus, the only possible energy exchange process is the heat transfer from the matrix to the particles and the particles serve as a internal chill. The dominant mechanism of energy transport in this sub-domain is diffusion.

2. MATHEMATICAL MODEL

The governing equations for the conservation of energy [5] are:

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \nabla \cdot [\lambda_m(T)\nabla T_m(x,t)] + q_V, \ \ m = 1, 2 \qquad (2.1)$$

where $c_m(T)$ is the specific heat per unit of volume, $\lambda_m(T)$ is the thermal conductivity, T, $x = \{x_1, x_2, x_3\}$, t denote the temperature, geometrical co-ordinates and time. Index $m = 1$ identifies the aluminum sub-domain and $m = 2$

identifies the lead sub-domain. The term q_V is the source function and this term can be written in the form

$$q_V = L_m \frac{\partial f_S(x,t)}{\partial t}, \quad m = 1,2 \tag{2.2}$$

where L_m is the latent heat per unit of volume, f_S is the solid state fraction at the neighborhood of considered point x. Pure metals (e.g. aluminum and lead) solidify at a constant temperature T^*. The function f_S changes from 0 (molten metal: for $T_m(x, t) > T_m^*$) to 1 (solid body: for $T_m(x, t) < T_m^*$). The value of $\lambda_m(T)$ is determined by relation

$$\lambda_m(T) = \begin{cases} \lambda_{Lm} & \text{for } T > T_m^* \\ (1 - f_S)\lambda_{Lm} + f_S \lambda_{Sm} & \text{for } T = T_m^*, \quad m = 1, 2 \\ \lambda_{Sm} & \text{for } T < T_m^* \end{cases} \tag{2.3}$$

where λ_{Lm}, λ_{Sm} are the thermal conductivities of the liquid and solid phases of the metals. In a similar way one can determine $c_m(T)$.

On the contact surface between matrix and particle the IV type of boundary condition is assumed

$$\begin{cases} -\lambda_1 \dfrac{\partial T_1(x,t)}{\partial n} = -\lambda_2 \dfrac{\partial T_2(x,t)}{\partial n} \\ T_1(x,t) = T_2(x,t) \end{cases} \tag{2.4}$$

where $\partial/\partial n$ denotes a normal derivative. On the external surface of the domain the II type of boundary condition in the form

$$\frac{\partial T_1(x,t)}{\partial n} = 0 \tag{2.5}$$

is given. For time $t = 0$ the initial conditions are also known

$$t = 0: \quad T_1(x,0) = T_{01} > T_1^*, \quad T_2(x,0) = T_{02} < T_2^* \tag{2.6}$$

3. NUMERICAL MODELING USING THE CONTROL VOLUME METHOD (CVM)

CVM [1, 2, 4-7] constitutes an effective tool for numerical computations of heat-transfer processes. The domain considered and its discretization are shown in Figure 3. One can see that the cubic control volumes (CV) are applied.

The CVM algorithm allows the transient temperature field to be found at the set of nodes corresponding to the central points of control volumes. The nodal temperatures can be determined on the basis of energy balances for successive volumes. Let us consider the control volume ΔV_i with central node x_i (see Fig. 3b). It is assumed here that the thermal capacities and capacities of internal heat sources are concentrated at the nodes representing elements, while the thermal resistances are concentrated at the sectors joining the nodes.
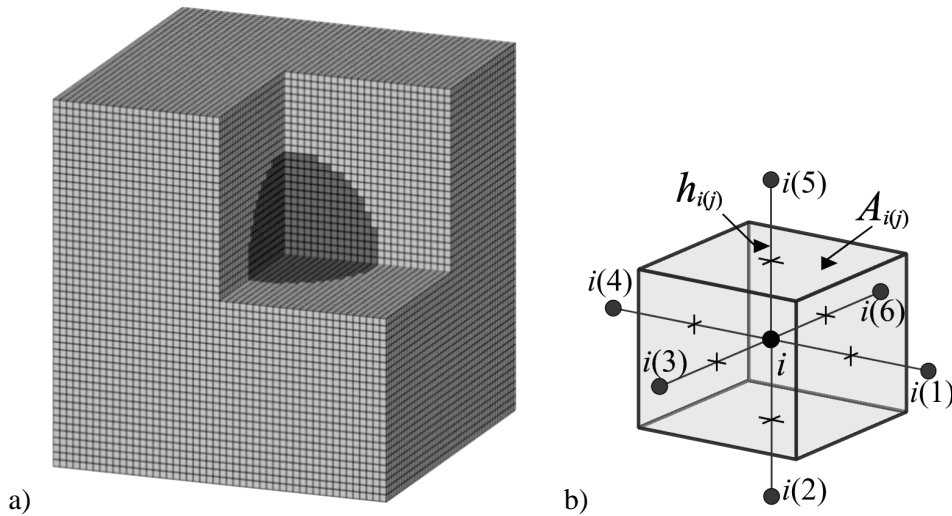

Fig. 3. a) Discretization of the domain considered with 50^3 control volumes
b) Control volume ΔV_i

3.1. Balance equations

The energy balance for the control volume ΔV_i can be written in the form [2,4,5]

$$\Delta H_i = \sum_{j=1}^{6} Q_{ij}^f + q_{V_i} \Delta V_i \Delta t \tag{3.1}$$

where Δt is the interval of time, $\Delta t = t^{f+1} - t^f$; $f, f+1$ denotes two successive time steps, Q_{ij}^f is the heat conducted at the time Δt from the adjoining nodes $x_{i(j)}$ to node x_i. We assume that the heat fluxes flowing to the ΔV_i are proportional to the temperature differences at the moment $t = t^f$, $(T_i^f = T(x_i, t^f))$, then we shall obtain a solving system of the type 'explicit scheme'. So

$$Q_{ij}^f = \frac{\left(T_{i(j)}^f - T_i^f\right)}{R_{ij}^f} A_{i(j)} \Delta t \tag{3.2}$$

where R_{ij}^f is the thermal resistance between points x_i and $x_{i(j)}$, $A_{i(j)}$ is area of the surface limiting the domain ΔV_i in direction $i(j)$. If we denote by $h_{i(j)}$ the distance between the nodes x_i, $x_{i(j)}$ then

$$R_{ij}^f = \frac{h_{i(j)}/2}{\lambda_i^f} + \frac{h_{i(j)}/2}{\lambda_{i(j)}^f} = h_{i(j)} \frac{\lambda_i^f + \lambda_{i(j)}^f}{2\lambda_i^f \lambda_{i(j)}^f} \tag{3.3}$$

where λ_i^f and $\lambda_{i(j)}^f$ are a mean thermal conductivities in the domains ΔV_i and $\Delta V_{i(j)}$ respectively, determined by formula (2.3). Another definition of thermal resistance should be introduced for the boundary volumes [5]. In order to take into account non-flux boundary condition (2.5) (in the case of external CV) we assume $R_{ij}^f = \infty$ (in numerical realization e.g. $R_{ij}^f = 10^{12}$) if the surface limiting the domain ΔV_i in the direction $i(j)$ is a part the boundary.

The term q_{Vi} in eq. (3.1) is approximated by relation

$$q_{V i} = L_i \frac{f_{S i}^{f+1} - f_{S i}^f}{\Delta t} \tag{3.4}$$

The change of enthalpy of control volume ΔV_i during the time Δt equals

$$\Delta H_i = c_i^f \left(T_i^{f+1} - T_i^f \right) \Delta V_i \tag{3.5}$$

where c_i^f is the volumetric specific heat similarly determined by formula (2.3).

The energy balance written in the convention of "explicit" scheme takes the form

$$c_i^f \left(T_i^{f+1} - T_i^f \right) \Delta V_i = \sum_{j=1}^{6} \frac{T_{i(j)}^f - T_i^f}{R_{ij}^f} A_{i(j)} \Delta t + L_i \left(f_{S i}^{f+1} - f_{S i}^f \right) \Delta V_i \tag{3.6}$$

from which

$$T_i^{f+1} = T_i^f + \frac{\Delta t}{c_i^f \Delta V_i} \sum_{j=1}^{6} \frac{T_{i(j)}^f - T_i^f}{R_{ij}^f} A_{i(j)} + \frac{L_i}{c_i^f} \left(f_{S i}^{f+1} - f_{S i}^f \right) \tag{3.7}$$

or

$$T_i^{f+1} = T_i^f + \sum_{j=1}^{6} W_j \left(T_{i(j)}^f - T_i^f \right) + \frac{L_i}{c_i^f} \left(f_{S i}^{f+1} - f_{S i}^f \right) \tag{3.8}$$

where

$$W_j = \frac{A_{i(j)}\,\Delta t}{c_i^f\,R_{ij}^f\,\Delta V_i} \tag{3.9}$$

The stability condition

$$1 - \sum_{j=1}^{6} W_j > 0 \tag{3.10}$$

allows to determine the critical time step

$$\Delta t < \left(\sum_{j=1}^{6} \frac{A_{i(j)}}{c_i^f\,R_{ij}^f\,\Delta V_i} \right)^{-1} \tag{3.11}$$

Initial conditions (2.6) are introduced as

$$
\begin{aligned}
& x_i \in \text{sub-domain Al}: \quad T_i^0 = T_{01}, \quad f_{S\,i}^{\,0} = 0 \\
& x_i \in \text{sub-domain Pb}: \quad T_i^0 = T_{02}, \quad f_{S\,i}^{\,0} = 1
\end{aligned}
\tag{3.12}
$$

3.2. Modeling of phase changes

Two unknown values T_i^{f+1} and $f_{S\,i}^{\,f+1}$ at the time $t = t^{f+1}$ occur in eq. (3.8). During the heating (cooling) processes proceeding in domain ΔV_i the following situations should be taken into account:

Case 1: If $T_i^f \neq T_i^*$ then it is assumed that $f_{S\,i}^{\,f+1} = f_{S\,i}^{\,f}$ and simultaneously T_i^{f+1} is calculated from eq. (3.8) – the last term in eq. (3.8) is equal to 0. In the case, where the calculated temperature T_i^{f+1} equals $T_i^{f+1} < T_i^*$ (for $T_i^f > T_i^*$) or $T_i^{f+1} > T_i^*$ (for $T_i^f < T_i^*$) then it is assumed that $T_i^{f+1} = T_i^*$, whereas the new value of $f_{S\,i}^{\,f+1}$ is calculated on the basis of eq. (3.8), as

$$f_{S\,i}^{\,f+1} = f_{S\,i}^{\,f} + \frac{c_i^f}{L_i}\left(T_i^* - T_i^f - \sum_{j=1}^{6} W_j \left(T_{i(j)}^f - T_i^f \right) \right) \tag{3.13}$$

The above relationship allows to start the solidification (melting) process at the constant temperature.

Case 2: If $T_i^f = T_i^*$ then it is assumed that $T_i^{f+1} = T_i^*$ and $f_{S\,i}^{\,f+1}$ is determined on the basis of eq. (3.8) (assuming $T_i^{f+1} = T_i^f = T_i^*$) as

$$f_{S_i}^{f+1} = f_{S_i}^{f} - \frac{c_i^{f}}{L_i} \sum_{j=1}^{6} W_j \left(T_{i(j)}^{f} - T_i^{*} \right) \tag{3.14}$$

If the calculated value of $f_{S_i}^{f+1}$ from eq. (3.14) is $f_{S_i}^{f+1} > 1$ then it is set $f_{S_i}^{f+1} = 1$ or if $f_{S_i}^{f+1} < 0$ then it is set $f_{S_i}^{f+1} = 0$. Next, the new value of T_i^{f+1} is calculated using eq. (3.8). In this way, the solidification (melting) process ends and at the same time starts cooling (heating) of metal.

4. EXAMPLES OF COMPUTATION

The system of metal matrix (Al) and lead particle (Pb) is considered. Thermo-physical parameters of sub-domains are equal to – for Al: $c_S = 2.916 \cdot 10^6$, $c_L = 3.07 \cdot 10^6$ J/(m³ K), $\lambda_S = 261$, $\lambda_L = 104$ W/(m K), $L = 1.053 \cdot 10^9$ J/m³, $T^* = 660$ °C, and for Pb: $c_S = 1.566 \cdot 10^6$, $c_L = 1.579 \cdot 10^6$ J/(m³ K), $\lambda_S = 30.7$, $\lambda_L = 24.4$ W/(m K), $L = 2.55316 \cdot 10^8$ J/m³, $T^* = 327$ °C. The initial temperature of matrix is $T_{01} = 700$ °C, the initial temperature of lead particle is $T_{02} = 20$ °C.

In the first example, it was assumed that the particle diameter is $d = 100$ μm, the volume fraction of the lead particle in the cube equals $fr = 10$ %, then the side of the cube is $l = 173.65$ μm – eq. (1.1). In Figure 6 the course of isotherms corresponding to section A (see Figure 4) for times $t = 0.01$, 0.05, 0.1 ms are shown. In Figure 5 the temperature histories at the selected points are presented. One can see that on the heating curves in the Pb sub-domains occurs a characteristic transition stops from the solid state to liquid one. Similar stops on the cooling curves in the Al sub-domains one can observe, too. The Figure 6 shows the changes of f_S at the same set of points.
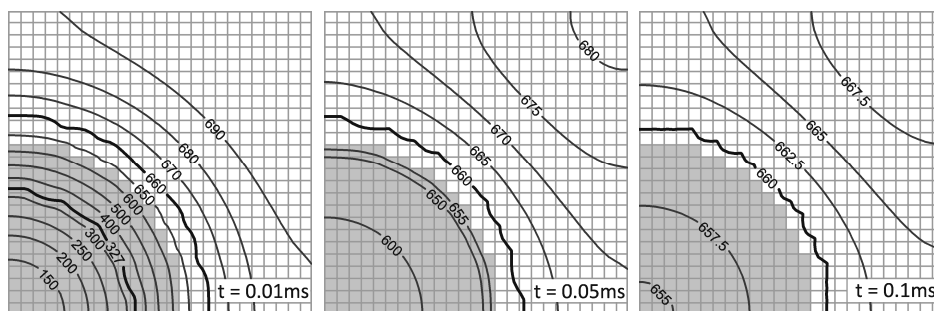

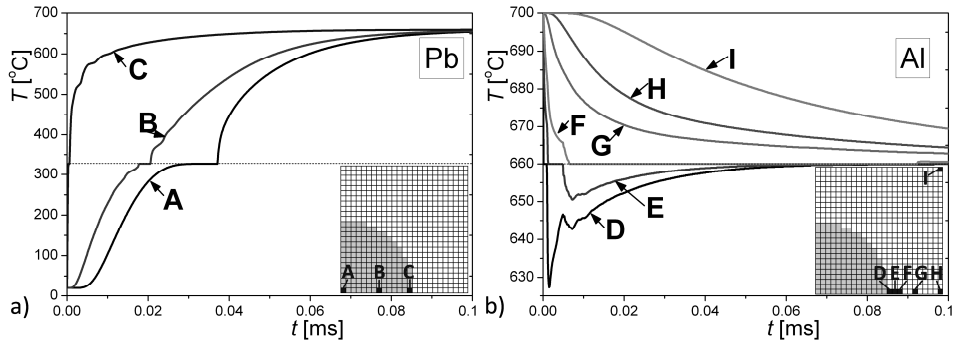Fig. 4. Courses of isotherms for different moments of time

Fig. 5. The profiles of temperature at the selected points
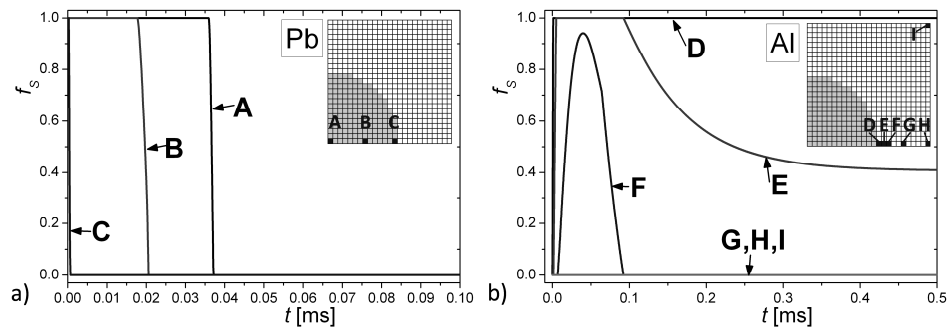a) in the Pb sub-domain,   b) in the Al sub-domain

Fig. 6. The changes of f_S at the set of points   (in Figure are different time-scales)
a) in the Pb sub-domain,   b) in the Al sub-domain

The second example concerns a study of influence of the volume fraction of lead particle on the thermal process in the system. For this purpose, numerical simulations for the following volumetric fractions of particle $fr = 10$, 20, 30 and 40 % have been calculated, assuming the constant diameter of particle $d = 100$ μm and the different sides of the cube $l = 173.65, 137.82, 120.40, 109.39$ μm respectively. The average temperature and average solid state fraction in Al and Pb sub-domains in cast composite are presented in Figure 7. One can observe that the heating lines and the solid state fraction lines in the Pb sub-domains are close to each other. One can conclude that total time of heating and melting of the Pb particle does not depend significantly on the volume fraction (for analyzed values) of surrounding Al matrix. This can be explained that the values of specific heat and the latent heat of aluminum are higher then heats of lead.
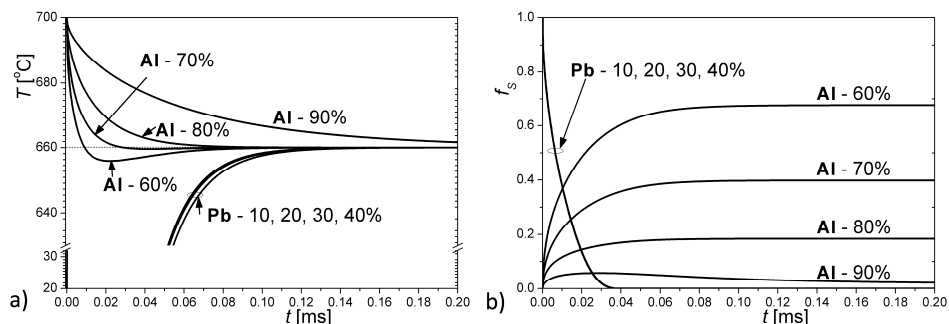
Fig. 7. The comparison of average temperature (a) and average solid state fraction (b)
in the Al and Pb sub-domains for different volume fractions of
sub-domains in composite

5. CONCLUSIONS

This paper presents the CVM algorithm which appears to be effective for the numerical modeling of thermal processes in the materials for which the solidification and the melting occur at constant temperatures.

Inside our composite system all thermal processes proceed in a very short time. In the early stage of heat exchange between the lead particle and the aluminum matrix the particle play a role of an internal chill. As a consequence in the vicinity of the particle's surface the matrix is under-cooled, i.e. its temperature is slightly below the freezing point. In this stage a thin film of solidified matrix appears and the particle is intensively heated. When the temperature of lead-particle exceeds the melting temperature there is a solid-to-liquid phase change. After this phase change the thickness of the solid aluminum film starts to decrease, however this thin-solid-layer has been observed during the simulation time. Finally, due to the non-flux boundary condition the temperatures of the system components equilibrate. The further stages of cooling are determined by the boundary conditions given on the outer surface of the casting but this process is not considered here.

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MODEL NUMERYCZNY KRZEPNIĘCIA KOMPOZYTU Z CZĄSTKAMI

S t r e s z c z e n i e

Praca dotyczy wymiany ciepła pomiędzy osnową i cząstkami tworzącymi materiał kompozytowy. W szczególności rozpatrywana jest objętość kontrolna (Al) w kształcie sześcianu, w którego środku umieszczona zostaje cząstka (Pb). Wymiary rozpatrywanej objętości kontrolnej zależą od gęstości cząstek wprowadzonych do osnowy. Założono, że objętość kontrolna umieszczona jest w centralnej części odlewanego kompozytu oraz, że warunki brzegowe zadane na powierzchni odlewu i formy nie wpływają na procesy cieplne w tej objętości. Oznacza to, że warunki przyjęte na powierzchniach granicznych sześcianu to warunki adiabatyczne. Równania różniczkowe i warunki brzegowe zapisano w konwencji entalpowej zakładając, że krzepnięcie osnowy i topnienie cząstek zachodzą w stałej temperaturze. Rozpatrywaną objętość kontrolną dzielono na 50^3 sześcianów. Do obliczeń numerycznych wykorzystano metodę bilansów elementarnych, przyjmując że pola temperatur w ciekłej osnowie i cząstce ołowianej są znane w chwili początkowej oraz, że kontakt między podobszarami układu jest idealny. W trakcie procesu obserwowano topnienie cząstki ołowianej i stygnięcie osnowy. W pracy przedstawiono wyniki symulacji numerycznych w postaci krzywych nagrzewania i stygnięcia w wybranych punktach obszarów, jak również przebieg izoterm w przekroju kompozytu dla kilku wybranych czasów. Ponadto zbadano wpływ zmian udziału objętościowego cząstki w osnowie na przebieg procesu wymiany ciepła.