Voronoi Tessellations Description of Cast Composite Solidification Processes

Zbigniew Domański, Mariusz Ciesielski, and Bohdan Mochnacki

***Abstract*—The paper presents a method to analyse the thermal processes occurring in the cast composite solidification. The domain of cast is formed by parallel fibres bundle randomly immersed in a host metal matrix. The heat is transferred from the metal matrix and absorbed by fibres. The objective of this paper is to evaluate the volumetric fraction of fibres for which the solidification of metal matrix occurs. Our method is to compute Voronoi diagrams with Voronoi regions representing the geometry location of the fibres in the metal matrix and to use these regions as control volume within a variant of Control Volume Method.**

***Index Terms*—cast composition solidification, heat transfer, Voronoi diagrams.**

I. Introduction

Heat conduction is a relevant topic in many industrial processes. Knowledge of the thermal conduction phenomena and its effective description are essential for the analysis of the heat transport processes occurring in heterogeneous media. An example of industrial importance is the solidification process of metal matrix composite (MMC) [1]–[7]. The formation of microstructures can be altered during the solidification process as is the case of fibre reinforced aluminium composite with the extended ends of the fibres cooled by a heat sink. MMC solidification has been investigated in various fibre arrangement scenarios including fixed inline or staggered fibre in a variety of spacing distributions. The presence of fibres has a reinforcing effect on mechanical properties of MMCs compared to monolithic metals. Superior mechanical, electrical and thermal properties of MMCs depend on the appropriate choice of the matrix and fibre materials, their shape and fabrication method.

The problem we consider is the solidification of the metal (the matrix) in the presence of fibres. The aim of our investigation is to determine the volumetric fraction of fibres for which the solidification of metal matrix proceeds in 'a natural way' due to the heat exchange between the matrix and fibres.

II. Mathematical Model

We consider a hypothetic process of the synthesis of MMC by casting. During this process the fibres do not undergo phase change because their melting temperature is much higher than that of the matrix. The solidifying matrix and fibres are contained within a cavity with adiabatic walls and the only possible energy exchange process is the heat transfer form the matrix to the fibres so the fibres serve as a heat sink. The dominant mechanism of energy transport in the cavity is diffusion.

The governing equations for the conservation of energy [8], including the presence of the fibres bundle are:

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

where $c_m(T)$ is the specific heat per unit of volume, $\lambda_m(T)$ is thermal conductivity, T, x, y, t denote the temperature, geometrical co-ordinates and time. Index $m = 1$ identifies the matrix sub-domain and $m = 2$ identifies the fibres sub-domain. The term q_V is the source function and this term can be written in the form

$$q_V = \begin{cases} L\dfrac{\partial f_S(x,y,t)}{\partial t}, & \text{for } m=1 \\ 0, & \text{for } m=2 \end{cases} \quad (2)$$

where L is the latent heat per unit of volume, f_S is the solid state fraction at the neighbourhood of the considered point (x, y). Pure metals (e.g. aluminium) solidify in a constant temperature T^*. The function f_S changes from 0 (molten metal: for $T_1(x, y, t) > T^*$) to 1 (solid body: for $T_1(x, y, t) < T^*$).

The value of $\lambda_m(T)$ is determined by relation

$$\lambda_m(T) = \begin{cases} \lambda_L & \text{for } m=1 \text{ and } T > T^* \\ (1-f_S)\lambda_L + f_S\lambda_S & \text{for } m=1 \text{ and } T = T^* \\ \lambda_S & \text{for } m=1 \text{ and } T < T^* \\ \lambda_{fib} & \text{for } m=2 \end{cases} \quad (3)$$

where λ_L, λ_S are thermal conductivities of the liquid and solid state of the metal matrix and λ_{fib} is the thermal conductivity of the fibres bundle. In a similar way one can determine $c_m(T)$.

On the contact surface between the matrix and fibre a continuity of temperature and a continuity of heat flux are assumed

$$\begin{cases} -\lambda_1\dfrac{\partial T_1(x,y,t)}{\partial n} = -\lambda_2\dfrac{\partial T_2(x,y,t)}{\partial n} \\ T_1(x,y,t) = T_2(x,y,t) \end{cases} \quad (4)$$

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

$$\frac{\partial T_m(x,y,t)}{\partial n} = 0 \tag{5}$$

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

$$t = 0: \quad T_1(x,y,0) = T_{10}, \;\; T_2(x,y,0) = T_{20} \tag{6}$$

III. Voronoi Tessellation and Mesh Generation

In a numerical modelling of the solidification process considered the metal-matrix and fibre sub-domains are divided into small cells (control volumes), known as the Voronoi polygons (also called the Thiessen or Dirichlet cells in two dimensions) [9]–[13]. The Voronoi polygons are one of the most fundamental and useful constructs defined by irregular lattices. For a set $\mathbf{X} = \{x_1, x_2, ..., x_N\}$ of N distinct points in $\mathbf{R}^2$, the Voronoi tessellation is the partition of $\mathbf{R}^2$ into N polygons. The polygon that contains point x_i (central point) is denoted by ΔV_i. Each region ΔV_i is defined as the set of points in $\mathbf{R}^2$ which are closer to x_i than to any points in $\mathbf{X}$:

$$\Delta V_i = \left\{ X \in \mathbf{R}^2 : d(X, x_i) < d(X, x_j), \forall j \neq i, \; j = 1, \ldots, N \right\} \tag{7}$$

where $d(\cdot,\cdot)$ is the Euclidean distance function. All of the Voronoi regions are convex polygons. In Fig. 2 the example of Voronoi polygons is shown. A single polygon is defined by the lines that bisect the lines between the central point and its surrounding points. The bisecting lines and the connection lines are perpendicular to each other. When we use this rule for every point in the area, the area will be completely covered by adjacent polygons. Some of them are infinite ("open") because they have no neighbouring points in that direction.

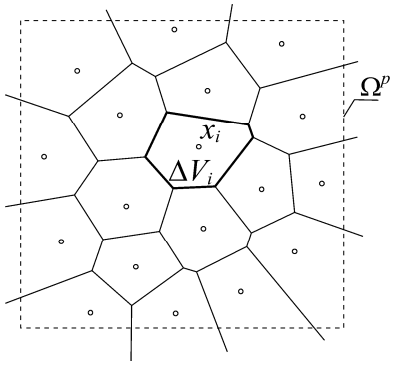

Fig. 1. The Voronoi polygons for a set of arbitrarily distributed points

Many algorithms to construct the Voronoi polygons can be found in literature. One popular method is based on the Delaunay triangulation [9]–[12]. This triangulation can be formulated in a circle criterion. The Delaunay triangulation DT of a set $\mathbf{X}$ of points in the plane is such a triangulation $DT(\mathbf{X})$ that consists of non-overlapping triangles and contains no points of $\mathbf{X}$ inside the circumcircle of any triangle in $DT(\mathbf{X})$. This triangulation is the dual structure of the Voronoi tessellation. The polygons are defined by lines that bisect the connection lines between neighbouring points and the centers of circumcircles are the vertices of the Voronoi polygons. In the case of unbounded polygons whose center points lie on the convex hull of set $\mathbf{X}$, they are bound by the boundaries of the domain Ω^p – see Fig. 1.

Positions of points in the set $\mathbf{X}$ are usually determined randomly and hence the mesh of control volumes is unstructured. We additionally impose the requirement that the minimal distance between two points must be greater than the pre-assigned value. It makes the polygons more uniform and the central point lies nearer the middle of the polygon.

In Fig. 2 an example of the structure of cast composites with 40% fibres is shown. The domain has been divided into 2351 control volumes. Gray control volumes determine the fibre sub-domain. If we assume the fibres bundle is parallel then on the section considered one obtains the discrete set of circles. The position of the fibre center $P_j = (x_{0j}, y_{0j})$, where j is an index of the fibre considered, is determined in a random way. Also the fibre radius r_j is randomly determined $r_j \in [r_{\min}, r_{\max}]$. The number of CV should assure a good approximation of fibre circular cross-sections. The positions of central points in CV close to the contact between fibre and metal-matrix are analytically determined in order to achieve a better approximation of the fibres shape. The geometrical parameters of a system matrix-fibres are chosen on the basis of the optical micrographs presented in [14]. It can be seen that the fibres diameters are different, and also their mutual positions are rather incidental. The only unquestionable information concerning the geometry of the system results from the volumetric fraction of the fibres in the domain analyzed. So, the numerical procedure realizing the mesh generation, fibres localization, values of fibres radii bases on the application of random numbers generation. On the stage of mesh generation, the type of sub-domain (m = 1, 2) for every CV is assigned.

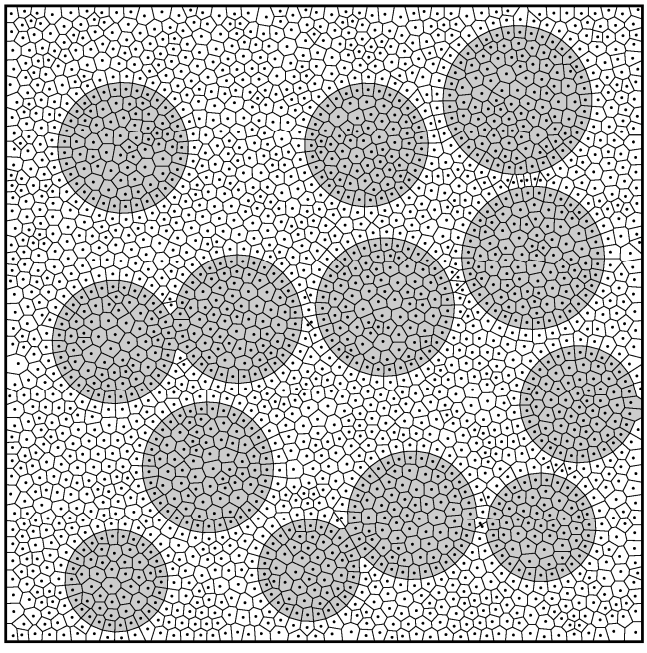

Fig. 2. Example of mesh

IV. Numerical Modelling

The control volume method (CVM) [8], [15]–[17] constitutes the effective tool for numerical computations of the heat transfer processes. The domain analyzed is divided into N volumes. The CVM algorithm allows to find the transient temperature field at the set of nodes corresponding to the central points of the control volumes. The nodal temperatures can be found on the basis of energy balances for the successive volumes. In order to assure the correctness and exactness of the algorithm proposed we generate the control volumes in the shape of the Voronoi polygons (see: Fig. 3).

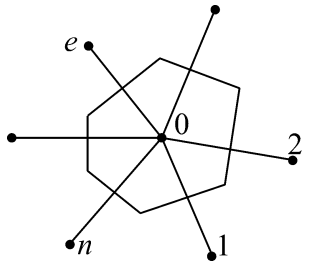

Fig. 3. Control volume ΔV_0

Let us consider the control volume ΔV_0 with the central node x_0. It is assumed here that the thermal capacities and capacities of the internal heat sources are concentrated in the nodes representing elements, while thermal resistances are concentrated in the sectors joining the nodes.

The energy balance for the control volume ΔV_0 can be written in the form

$$\Delta H_0 = \sum_e Q_e + |\Delta V_0| q_V \Delta t \tag{8}$$

where ΔH_0 is a change of control volume enthalpy during the time interval Δt, Q_e – the heat conducted at the time Δt from the adjoining nodes to the node x_0, q_V – a mean capacity of internal heat sources in the control volume ΔV_0.

If one assumes that the heat fluxes flowing to the element ΔV_0 are proportional to the temperature differences at the moment $t = t^f$, then we shall obtain a solving system of the type 'explicit scheme'. So

$$Q_e = \frac{T_e^f - T_0^f}{R_{0e}^f} \Delta A_e \Delta t \tag{9}$$

where R_{0e}^f is the thermal resistance between points x_0 and x_e [8], ΔA_e surface limiting the domain ΔV_0 in the direction e. If we denote by h_e the distance between the nodes x_0 , x_e then

$$R_{0e}^f = \frac{h_e}{2\lambda_0^f} + \frac{h_e}{2\lambda_e^f} \tag{10}$$

where λ_0^f and λ_e^f are the thermal conductivities in the control volumes ΔV_0 and ΔV_e at the moment $t = t^f$. The other definition of thermal resistance should be introduced for the boundary volumes [8]. For the boundary condition (5) we assume $R_{0e}^f = \infty$ (in numerical realization e.g. $R_{0e}^f = 10^{10}$) if the surface limiting the domain ΔV_0 in the direction e is a part of the boundary - it assures to zero heat flux in the direction e.

The change of enthalpy of the control volume ΔV_0 during the time Δt equals [8], [15]

$$\Delta H_0 = c_0^f \left(T_0^{f+1} - T_0^f\right) |\Delta V_0| \tag{11}$$

where c_0^f is the volumetric specific heat, f, f+1 denotes two successive time levels.

Let us write the balance equation in the explicit scheme

$$c_0^f \left(T_0^{f+1} - T_0^f\right) |\Delta V_0| = \sum_e \frac{T_e^f - T_0^f}{R_{0e}^f} \Delta A_e \Delta t + |\Delta V_0| q_V \Delta t \tag{12}$$

or

$$T_0^{f+1} = \sum_{e=0}^{n} W_e T_e^f + \frac{q_V \Delta t}{c_0^f} \tag{13}$$

where

$$W_e = \frac{\Delta t \, \Delta A_e}{c_0^f R_{0e}^f |\Delta V_0|}, \quad e = 1,\ldots,n \tag{14}$$

$$W_0 = 1 - \sum_{e=1}^{n} W_e \tag{15}$$

In order to assure the stability of the above explicit scheme the coefficient W_0 must be positive.

Next, the problem of metal solidification in the control volume ΔV_0 in a constant temperature T^* will be discussed. Let us assume that at the time $t = t^f$ the temperature T_0^f in node x_0 is $T_0^f > T^*$ (the molten metal), and the calculated temperature $T_0^{f+1} < T^*$. The change of enthalpy for ΔV_0 during the time Δt is as follows

$$\Delta H_0 = c_0^f \left(T_0^f - T_0^{f+1}\right) |\Delta V_0| \tag{16}$$

The enthalpy ΔH_0 can be divided into two components

$$\Delta H_{01} = c_0^f \left(T_0^f - T^*\right) |\Delta V_0|, \quad \Delta H_{02} = \Delta H_0 - \Delta H_{01} \tag{17}$$

The change of enthalpy ΔH_{02} associated with the solidification of the control volume ΔV_0 is equal to

$$\Delta H_{02} = L \, \Delta f_{S0}^{f+1} |\Delta V_0| \tag{18}$$

where $\Delta f_{S0}^{f+1} |\Delta V_0|$ is a solidified part of the considered volume ΔV_0. So, the energy balance for ΔV_0 in which the solidification process starts, can be written in the form

$$c_0^f \left(T_0^f - T_0^{f+1}\right) |\Delta V_0| = c_0^f \left(T_0^f - T^*\right) |\Delta V_0| + L \, \Delta f_{S0}^{f+1} |\Delta V_0| \tag{19}$$

From the last equation one obtains

$$\Delta f_{S0}^{f+1} = \frac{c_0^f \left(T^* - T_0^{f+1}\right)}{L} \tag{20}$$

and simultaneously

$$f_{S0}^{f+1} = \Delta f_{S0}^{f+1}, \quad T_0^{f+1} = T^* \tag{21}$$

If in the control volume ΔV_0 the first portion of solid metal is present then it is assumed that the temperature corresponding to ΔV_0 equals T^* and for the successive steps of time the following difference equation is required

$$\sum_e \frac{T_e^f - T_0^f}{R_{0e}^f} \Delta A_e \Delta t + L\left(f_{S0}^{f+1} - f_{S0}^f\right)\left|\Delta V_0\right| = 0 \tag{22}$$

From the last equation one obtains

$$f_{S0}^{f+1} = f_{S0}^f + \frac{\Delta t}{L\left|\Delta V_0\right|} \sum_e \frac{T_0^f - T_e^f}{R_{0e}^f} \Delta A_e \tag{23}$$

whereas $T_0^{f+1} = T^*$. For the one of successive steps of time it turns out that $f_{S0}^{f+1} > 1$, this means that more than the whole ΔV_0 has solidified. The enthalpy connected with this factious solidification of ΔV_0 above $f_S = 1$ should be recalculated on the enthalpy connected with cooling of the solid state

$$L\left(f_{S0}^{f+1} - 1\right)\left|\Delta V_0\right| = c_0^f \left(T^* - T_0^{f+1}\right)\left|\Delta V_0\right| \tag{24}$$

hence

$$T_0^{f+1} = T^* - \frac{L\left(f_{S0}^{f+1} - 1\right)}{c_0^f}, \quad f_{S0}^{f+1} = 1 \tag{25}$$

In the successive steps of time the energy balance for ΔV_0 is of the form (13).

V. Example of Computations

Numerical simulations of a casting process have been executed for the matrix-fibre (pure metal *Al*) with thermophysical parameters: $c_S = 2.943 \cdot 10^6$, $c_L = 3.07 \cdot 10^6$ J/(m^3 K), $\lambda_S = 261$, $\lambda_L = 104$ W/(m K), $L = 1.053 \cdot 10^9$ J/m^3, $T^* = 660$ °C, initial temperature $T_{10} = 700$ °C and the fibres (*Si*) with thermophysical parameters: $c_{fib} = 1.63 \cdot 10^6$ J/(m^3 K), $\lambda_{fib} = 148$ W/(m K), initial temperature $T_{20} = 20$ °C. The considered domain (2D problem) has the dimension 100 μm × 100 μm. In simulations the fibres fraction has been assumed as 40%, 50% and 55%.

In Figures 4, 5 and 6 the kinetics of the solidification process for different fibres fraction are presented. The influence of fibres fraction, initial temperatures of sub-domains considered on solidification time is very essential. In the case of the simulation with the 55% of fibres fraction, the whole liquid metal passes to the solid state without external thermal interactions. The algorithm proposed allows to analyze the thermal processes in a system matrix-fibres for the different technological conditions (fraction of fibres, initial temperatures, boundary conditions etc.).

From the enthalpy balance approach (for adiabatic system) one can determined in an analytical way fibres fraction for which the whole liquid metal passes to the solid state. The enthalpy balance can be written as follows

$$(1 - fr) \cdot H_1(T_{10}) + fr \cdot H_2(T_{20}) = \overline{H}(T^*) \tag{26}$$

where *fr* is fibres fraction in the considered domain, H_1 and H_2 are enthalpies of metal-matrix and fibre sub-domains respectively and $\overline{H}$ is enthalpy of the whole domain. Assuming that $T_{10} > T^*$ then the enthalpy H_1 is defined by

$$H_1(T_{10}) = \int_{T_{ref}}^{T^*} c_S \, d\tau + L + \int_{T^*}^{T_{10}} c_L \, d\tau \tag{27}$$

and the enthalpy H_2 equals to

$$H_2(T_{20}) = \int_{T_{ref}}^{T_{20}} c_{fib} \, d\tau \tag{28}$$

Assuming that the whole liquid metal passes to the solid state and final established temperature of the whole domain (the metal matrix sub-domain and fibres sub-domain) is equal to T^*, then the enthalpy $\overline{H}$ is defined by

$$\overline{H}(T^*) = (1 - fr) \int_{T_{ref}}^{T^*} c_S \, d\tau + fr \int_{T_{ref}}^{T^*} c_{fib} \, d\tau \tag{29}$$

Substituting (27), (28) and (29) into (26) and assuming that c_L, c_S, c_{fib} are constant, one can calculate the value *fr*

$$fr = \frac{L + c_L \left(T_{10} - T^*\right)}{L + c_L \left(T_{10} - T^*\right) + c_{fib} \left(T^* - T_{20}\right)} \tag{30}$$

For the above thermophysical parameters we obtain the value $fr = 52{,}98\%$. This analytical result confirms the correctness of numerical results.

VI. Conclusion

In the present work, the Voronoi diagrams have been exploited to generate a family of meshes for the control volume method algorithm. The properties of Voronoi diagram permit to find the nodal temperatures in an effective manner. When the cast solidifies the shapes of solidified domains changes in a peculiar manner around the cooling fibres. Thus, the random Voronoi tessellations allow to achieve higher correspondence with the temperature field than widely used regular tessellations. While the method is presently limited to rather simple, circular-fibre-shapes, work

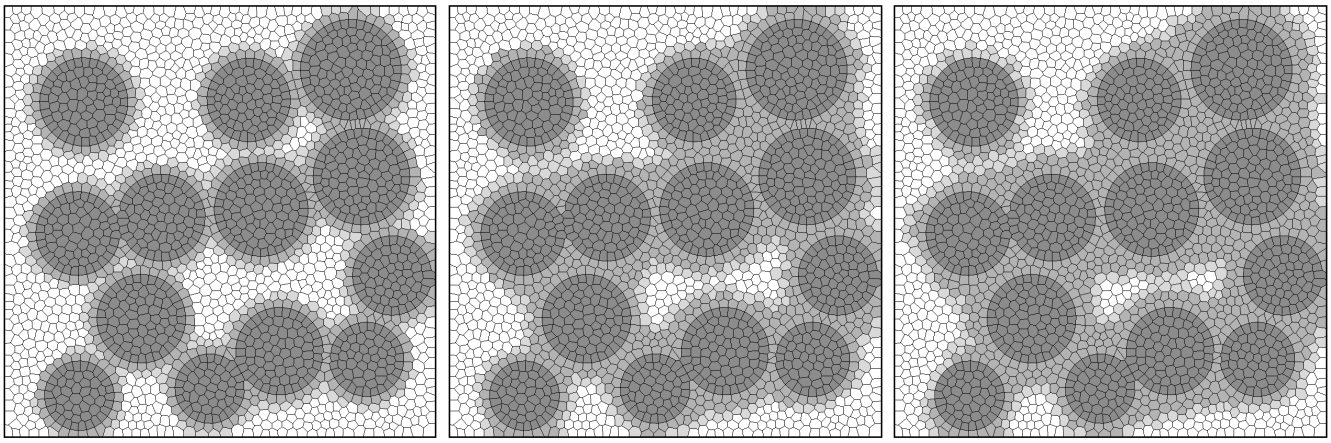

Fig. 4. The kinetics of solidification – 40% fibres fraction

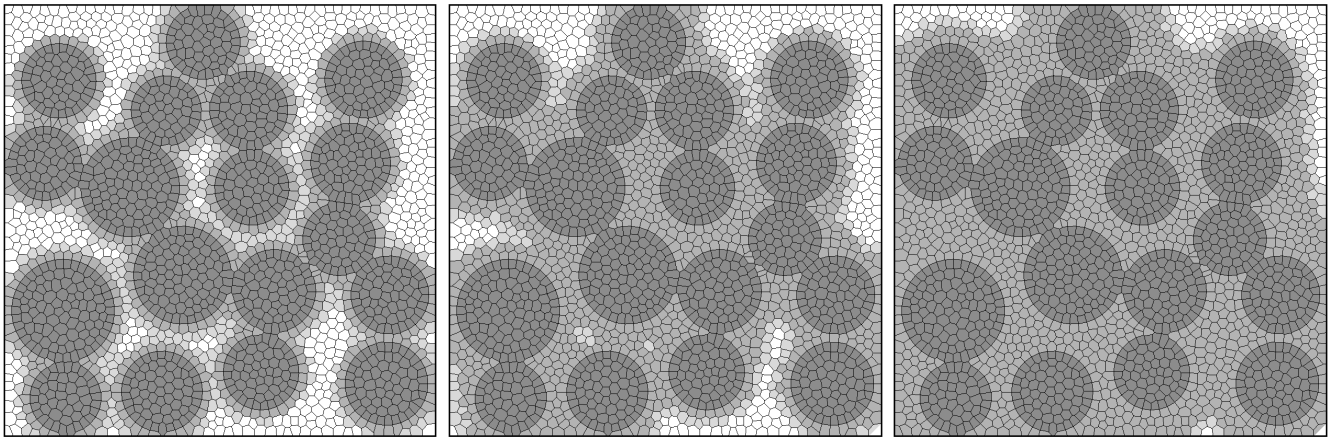

Fig. 5. The kinetics of solidification – 50% fibres fraction

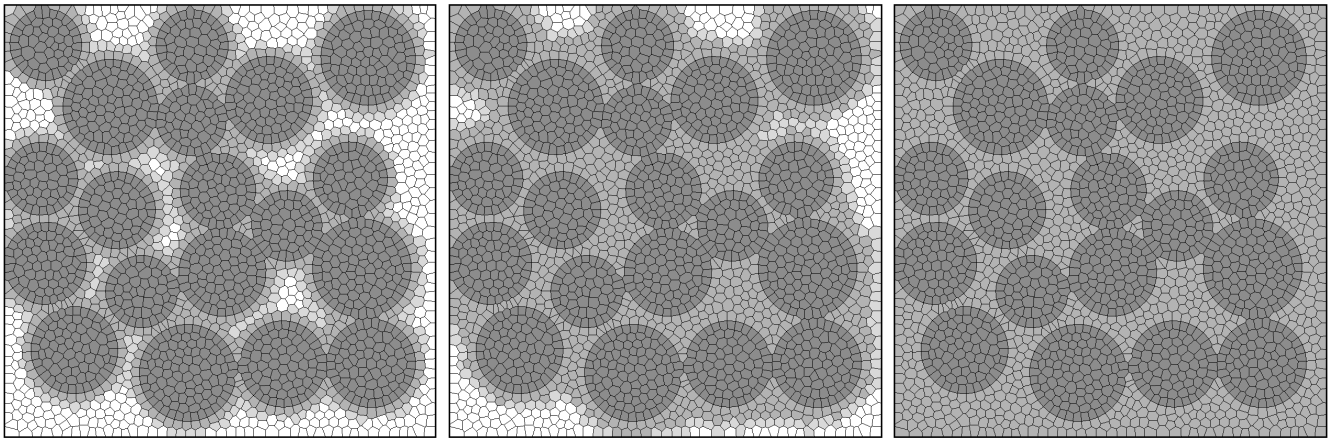

Fig. 6. The kinetics of solidification – 55% fibres fraction

is presently in progress to extend it to fibres with noncircular cross-sections and to metal matrix composites with random orientations of cooling fibres.

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