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THE MULTI-SCALE APPROACH TO NUMERICAL MODELLING OF SOLIDIFICATION

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ABSTRACT

The solidification process of pure metals or alloys can be modelled numerically using the macro models (the 1st generation models) and micro models (the 2nd generation models) [1]. The difference between macro and micro/macro models consists in the way of source function modelling. In the micro models the microstructure evolution (nucleation and nuclei growth) during the solidification process is considered. Nucleation begins when the local temporary temperature T decreases below the solidification point T^*. The process stops when the temperature T begins to increase and then the number of nuclei achieves a maximum value. After the nucleation, the grains radii increase continuously until the volume of solid state fills the whole volume of casting domain. The changes of temporary volumetric fraction of solid at the considered point from casting domain result from the laws determining the nucleation and nuclei growth. In this paper the model of crystallization process based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) theory [1, 2] is taken into account. The kinetics of nucleation and nuclei growth is proportional to the undercooling $\Delta T = T^* - T$. The solid phase growth (equiaxial grains) is determined by formula $dR/dt = \mu \Delta T^2$, where R is a grain radius and μ is the growth coefficient. The number of nuclei N is calculated from relation $N = \Psi \Delta T^2$, where Ψ is the nucleation coefficient.

In order to solve the problem the control volume method (CVM) [2-5] has been used. The casting domain is covered by the regular mesh (e.g. in the shape of squares) macro-cells. In every macro-cell randomly set of central points is generated and next the mesh of control volumes (CV) is created. The CV correspond to the final shapes of grains (in other words, to the primary structure of the casting) and they are approximated by the Thiessen polygons (2D task) [3-5]. The number of control volumes (or number of nuclei) in macro-cell depends on the maximum undercooling T_{max} below T^*. This number is estimated on the basis of preliminary simulation with redundancy number of CV in order to determine average T_{max} in every macro-cell. Heat flux between two neighbouring macro-cells is transmitted through internal boundaries. For every internal boundary at every computational time step the heat flux flowing through these boundaries is calculated. The heat flux is determined on the basis of temperature difference at the CV that are adjacent to boundary. In this way specified heat fluxes (internal and external) constitute the boundary conditions for macro-cells at the next computational time step. For every micro control volume filling macro-cell the changes of temperature are determined by the

CVM alghoritm [4]. At every computational time step the average temperature T_{avg} in macro-cell is calculated. If $T_{avg} < T^*$ then the number of nuclei is calculated from the formula $N = \Psi \Delta T^2$. In the case of difference between present and previous number of nuclei, the CV (only from undercooled and non-grained) are chosen in a random way and grains growth in these CV is begun. The growth of grain causes the increase of the solid fraction f_S and change of the source term q_V in the CV. The process of nucleation will go on until the all CV in macro-cell will be grained.

As the example of numerical simulation, the aluminium bar (2D task) with dimensions 0.01[m] x 0.01[m] has been considered. The domain has been divided into 100 macro-cells. The substitute heat transfer coefficient $\alpha = 100$ [W/(m^{2}K)] (the Robin's boundary condition) at the bottom boundary has been assumed, at the same time the non-flux boundary conditions at the other boundaries have been applied. For the metal we assume: $\mu = 3 \cdot 10^{-6}$ [m/(s K^2)], $\Psi = 10^{11}$ [grains/(m^3 K^2)].

In Figure 1a the size of grains after the time 30s are shown. In Figure 1b the cooling curves (the average temperature) in the selected macro-cells in casting domain are presented. In Figure 1c zoom of nucleation phase from Figure 1b and number of created nuclei (sum over all macro-cells) are shown.

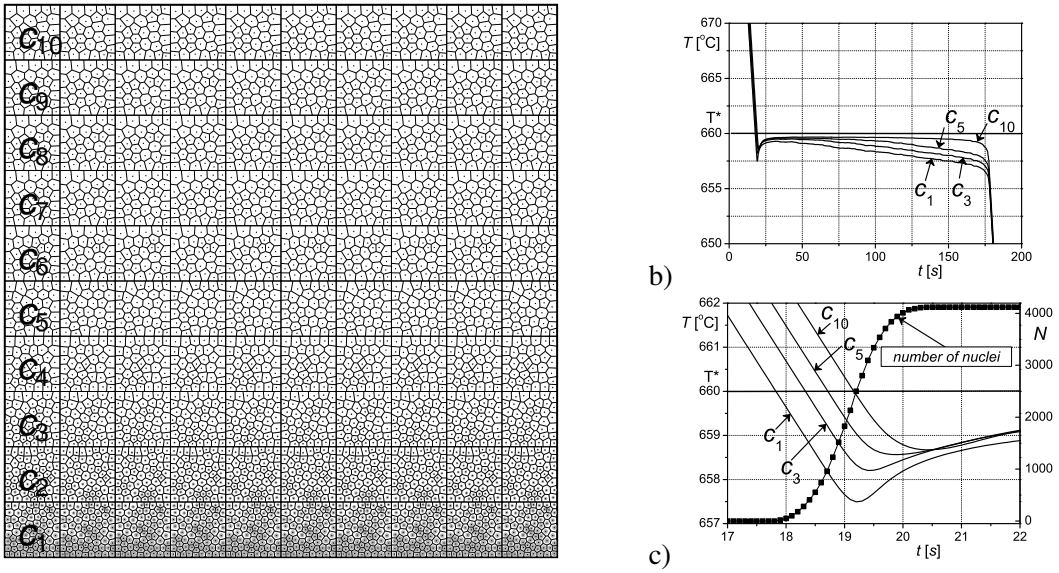

Figure 1: Example of local primary structure after 30s (a), the cooling curves in macro-cells c_1, c_3, c_5 and c_{10} (b), zoom of nucleation phase and number of created grains (c)

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