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GENERALIZED MICRO/MACRO MODEL OF CRYSTALLIZATION AND ITS NUMERICAL REALIZATION

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ABSTRACT

In the paper the considerations concerning the mathematical micro/macro model of pure metals solidification are presented. In particular the generalized approach close to the Mehl-Johnson-Avrami-Kolmogoroff theory (e.g. [1]) is applied. On a stage of numerical simulation the course of nucleation and nuclei growth are simulated according to the procedure described in [2]. Obtained in this way the local capacities of internal heat sources are taken into account in numerical solution of macro problem described by the Fourier-type equation.

The heat transfer processes proceeding in the solidifying casting volume (only heat conduction is taken into account) are described by the following energy equation [2]

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] + L\frac{\partial f_S(x,t)}{\partial t} \tag{1}$$

where $c(T)$ is a volumetric specific heat, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, f_S is a volumetric solid state fraction at the point considered, T, x, t denote the temperature, spatial coordinates and time. The equation (1) is supplemented by the adequate boundary and initial conditions (more complex models of take also into account the thermal processes proceeding in the mould subdomain).

The micro/macro models of solidification discussed below require the introduction of the function being the product of nuclei density N [nuclei/m^3] and single grain volume V [m^3], namely [1]

$$\omega(x,t) = \frac{4}{3}\pi\nu N(x,t)\left[\int_0^t u(\tau)\mathrm{d}\tau\right]^3 \tag{2}$$

where $u = \partial R/\partial t$ is a crystallization rate (R is a grain radius), ν is a coefficient equals 1 in case of spherical grains or $\nu < 1$ (e.g. dendritic growth).

The function f_S appearing in equation (1) can be described in the following way [3]

$$\frac{\mathrm{d}f_S(\omega)}{[1-f_S(\omega)]^n} = \mathrm{d}\omega \tag{3}$$

For $n = 0$ and $n = 1$ the solutions of (3) fulfilling the condition $\omega = 0$: $f_S = 0$ leads to the well known linear and exponential models, correspondingly, but the others solutions (e.g. $n = 2$) can be also taken into account. These generalized models can be called the power-type ones and they can be useful for description of crystallization process and modelling of source term in equation (1).

We assume that the 'driving force' of crystallization is an undercooling below the solidification point T^* (a pure metal solidification is considered). In particular

$$N(x,t) = \Psi \Delta T^2(x,t) \tag{4}$$

where Ψ is a nucleation coefficient, ΔT - undercooling below a solidification point) is taken into account. It was assumed that the nucleation stops at maximum undercooling. The nuclei growth is determined by the following formula

$$u(x,t) = \frac{\mathrm{d}R(x,t)}{\mathrm{d}t} = \mu_1 \Delta T^2(x,t) + \mu_2 \Delta T^3(x,t) \tag{5}$$

where R is a grain radius and μ_1, μ_2 - growth coefficients.

Let us consider the control volume ΔV_i from an interior of the casting area. During a certain interval of time the temperature at central point of ΔV_i decreases below the solidification point and the crystallization process starts. We find the number of the first 'portion' of nuclei N_i^1 (using equation (4)) and the final radius of grains ΔR_i^1 (formula (5)). Next we determine the fraction f_S for control volume considered. In the next loop of computations we find N_i^2 and ΔR_i^2 and new local value of f_S remembering that the first grains generation N_i^1 has the radius $\Delta R_i^1 + \Delta R_i^2$, while the second generation $N_i^1 - N_i^2$ has the radius ΔR_i^2 . The similar procedure is continued during the next loops of computations. In this way we can to observe the growth of successive families of grains and to predict the primary structure of casting.

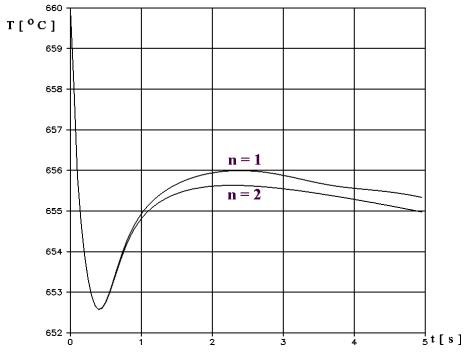

Figure 1: Cooling curves

As an example the solution obtained for aluminium plate (G/2=0.01m) produced in typical sand mould will be shown. The input data concerning the materials can be found in literature. In Figure 1 the cooling curves at the axis close to the plate boundary are shown (on the stage of computations the FDM has been used). They correspond to parameters $n = 1$ (Kolmogoroff model) and $n = 2$ (power-type model). Then

$$n = 2 : f_S = 1 - \frac{1}{\omega + 1} \tag{6}$$

The differences between the results obtained are not big, but visible. The optimal choice of n requires the experimental researches.

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