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Cellular automata for simulation of dendritic growth with surface active refractory inoculants

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ABSTRACT

Purpose: During weld metal structure formation the possibility of impact on its mechanical properties are much more limited in comparison with metallurgy and technology of steel production. Adding of the inoculants to the welding pool is one of the promising methods of influencing the structure and mechanical properties of the weld metal.

Design/methodology/approach: Cellular automata (CA) with additions of finite difference method (FDM) is one of the best ways to simulate dendritic growth process with the surface-active inoculants. It`s easy to add new rules of interaction between the inoculants and dendrite surface to the cellular automata model.

Findings: It was found that average distance between primary dendrites axis decrease with increase of the inoculants wetting angle by melt iron. Obtained results were confirmed experimentally on weld metal samples that were obtained by the welding of HSLA steels with the surface-active inoculants.

Research limitations/implications: The inoculants with size that comparable with cells size of the model (≈0.4 microns) were distributed evenly in computational area.

Practical implications: Adding of surface-active inoculants to the melt metal improve structure and mechanical properties of weld metal. Different refractory particles (TiC, TiN, SiC, TiO_2, Al_2O_3 and ZrO_2) can be used.

Originality/value: Refractory inoculants adding to the melt metal are wide used in metallurgy as crystallization centers and heat absorbers. Inoculants that were added to the welding pool of high-strength low-alloyed (HSLA) steel welds could also influence on crystallization processes of weld metal as surface active particles. In the contact point between the dendrite surface and the surface-active inoculant, a surface energy is change depending of the inoculant surface properties. Different refractory particles (TiC, TiN, SiC, TiO_2, Al_2O_3 and ZrO_2) were used.

Keywords: Solidification, Dendritic growth, Cellular automata, Simulation, Inoculants

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ANALYSIS AND MODELLING

1. Introduction

Main tendencies of high-strength low-alloy (HSLA) steels properties optimization are: reduction of alloying elements content, total number of micro-alloying elements increasing, content of additives and residual elements decreasing, structural homogeneity improvement, mechanical properties development [1].

Adding of refractory inoculants to the melt metal is a perspective method for optimizing structure and properties of HSLA steels due to regulation of structure and mechanical properties. It is well known that grain size of the primary structure effects on γ→α transformation. In case of disperse primary structure nucleation of α-phase starts from grain boundaries in the upper area of bainite transformation. In case of large dendrites nucleation of α-phase starts inside the primary grains at boundaries with non-metallic inclusions at the temperatures close to the end bainite transformation [2].

Work [3] considers a review and critical analysis of primary structure development models in point of view for application possibility for simulation of metal solidification process and account of the disperse refractory inoculants effect on solidification process. Present work proposes a model based on cellular automata method coupled with finite difference element method for simulation of the melt metal solidification with refractory inoculants.

2. Summary of the solidification model

Metal solidification process with the refractory inoculants can be considered as a result of two competing processes: high-rate movement of solidification front caused by local non-equilibrium of diffusion processes at phase interface [4,5], and effect of the refractory inoculants on the phase interfaces local surface energy [6].

Solution of this problem in present work is based on a model of local non-equilibrium solidification [7], which was supplemented by a model of solidification front interaction with the refractory inoculants. The model taken as a basis is used for small as well as high rates of solidification. Theoretical grounds of this model were made in work [8].

In two-dimensional space the equations of the solidification model [7] describe a mass balance (1), evolution of solid and liquid phase interface and diffusion flow of impurity (2, 3), growth of a solid phase (4) and relationship of impurity concentration in liquid and solid phases (5).

$$\frac{\partial}{\partial t}[(1-G)C_L + kGC_L] + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = 0, \tag{1}$$

$$\frac{\partial J_x}{\partial t} + J_x + \frac{1-G}{q}\frac{\partial C_L}{\partial x} = 0, \tag{2}$$

$$\frac{\partial J_y}{\partial t} + J_y + \frac{1-G}{q}\frac{\partial C_L}{\partial y} = 0, \tag{3}$$

$$\frac{\partial G}{\partial t} = \frac{\omega}{\upsilon}V, \tag{4}$$

$$C_S = kC_L, \tag{5}$$

where J_x and J_y are the projections of vector J of diffusion flow on coordinate axis; C_L and C_S are the concentration in liquid and solid phases, respectively; G is the fraction of solid phase in a cell [0...1]; t is the time; w is the area of phase interface in solidifying system; v is the volume of two-phase area; V is the rate of movement of intergrain boundary (interface of solid and liquid phases) along normal-vector directed to liquid phase side; k is the coefficient of the impurity non-equilibrium distribution.

Main assumptions of the model:

1. Isothermal two-phase system with constant pressure is considered.
2. The system consists of chemically inert binary alloy, which solidifies from undercooled liquid.
3. Freezing from liquid phase can be so fast that rate V of phase interface movement is compared on value with diffusion rate V_D of the impurity.
4. Convection in liquid phase and diffusion in solid phase are neglected.
5. Refractory inoculants are present in the liquid phase.
6. It is accepted that the refractory inoculants are evenly distributed in the weld pool.
7. Refractory inoculants are stationary during solidification. All inoculants have similar size, comparable with size of computational network cell (≈0.4 mm).

3. Basics of computational algorithm

A calculation area (solidification zone) is initiated at the beginning of calculation. It consists of solid phase of specific morphology and liquid phase with determined concentration of the impurity. A level of cell solidification is determined by fraction of solid phase in cell G. Each cell of the system can be liquid ($G = 0$) or completely solidified ($G = 1$), or belong to solidification front ($0 < G < 1$), i.e. freeze in a present moment of time (Fig. 1).

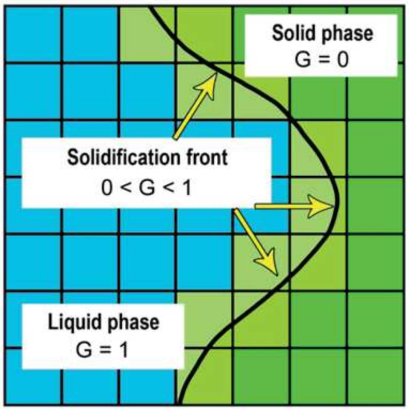

Fig. 1. Value of fraction of solid phase G for liquid and solid phases and solidification front

To determine an increment of solid phase fraction G it is necessary to calculate rate V of phase interface. This should be done with the help of non-linear kinetic equation «rate-undercooling»:

$$V = \beta(\Delta T - \Delta T_C(V) - \Delta T_N(V) - \Delta T_\Gamma), \quad (6)$$

where β is the kinetic coefficient of growth; ΔT is the complete initial undercooling in the system; ΔT_C is the concentration undercooling caused by the impurity diffusion; ΔT_N is the undercooling caused by change of inclination of kinetic liquidus and determined by difference between equilibrium line of liquidus and kinetic liquidus; ΔT_Γ is the undercooling caused by curvature of phase interface (Gibbs-Thompson`s effect). Details about influence of the different undercooling and boundary conditions of the model are considered in works [7-9].

4. Effect of the refractory inoculants on solidification process

Experimental data analysis [2,6] allowed taking a hypothesis for computations assuming that the solidification front absorbs the inoculant and surface tension in zone of contact is changed at the moment of contact.

To consider the effect of the refractory inoculants on solidification front movement it is necessary to compute a value of interphase tension between the inoculant and melt (σ_{12}) using data from [10].

$$\sigma_{12} = \sigma_1 + \sigma_2 - W_a, \quad (7)$$

where σ_{12} is the value of interphase tension between the refractory inoculant and melt metal; σ_1 is the inoculant surface tension; σ_2 is the alloy surface tension; W_a is the adhesion work.

Surface tension of the melt metal is computed based on procedure proposed by S. Popel [11]:

$$\sigma_2 = \sigma_{Fe} - 2000 \cdot lg \sum F_i x_i, \quad (8)$$

where σ_{Fe} is the surface tension of pure iron; F_i is the parameter characterizing capillary activity of alloying additive; x_i is the atomic fraction of i-th alloy component.

The boundary conditions are considered in work [9].

Software for tracing the movement of HSLA steels melt metal solidification front in time was developed on the model described above. The software inputs are initial conditions (initial solidification rate, initial morphology of solid phase, inclination angle of a vector of the most intensive heat rejection to solidification surface) and physical parameters of alloy (solidification temperature of alloy main component, growth kinetic coefficient, tangent of inclination angle of liquidus equilibrium line, equilibrium coefficient of additive distribution, coefficient of additive diffusion, solidification latent heat, rate of additive diffusion in volume and on phase interface, stochastic noise amplitude).

Based on developed software a series of computational experiments was carried out, the results of which are given below.

5. Melt metal composition influence on solidification process

Composition of the HSLA steel weld metal (wt.%): 0.049 C; 0.298 Si; 1.39 Mn; 0.023 S; 0.015 P; 0.15 Cr; 2.26 Ni; 0.25 Mo; 0.039 Al; 0.008 Ti was taken as a basis for computational experiments. Initial rate of solidification was accepted $0.27V_D$. Physical parameters of alloy are given in work [9]. Figure 2 shows difference in size and morphology of dendrites, which were developed for similar period of time, without considering the effect of alloying elements on alloy surface tension (Fig. 2a) and taking into account the effect alloying elements (Fig. 2b).

a) b)

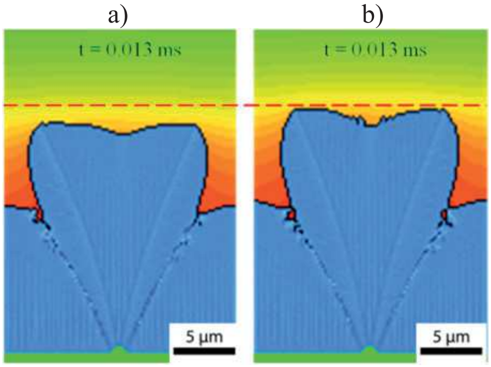

Fig. 2. Results of computations of solidification start: a – without effect of alloying elements; b – with alloying elements

6. Computational experiments results of the refractory inoculants introduction effect on dendrite structure

Titanium dioxide (TiO_2) was taken as introduced inoculant for the computations. It has the following parameters of surface interaction with iron melt: melting temperature (T_m) 1834°C; surface tension (σ_1) 1780 mJ/m^2; wetting angle (θ)≈0 degrees; adhesion work (W_a) 3560 mJ/m^2. A parameter of refractory inoculants distribution in the weld pool metal φ was taken equal 0, 0.1, 0.2, and 0.3. The results of computations showing evolution of the dendrite structure in time with different density of the inoculants distribution in the melt metal are given in Figures 3.

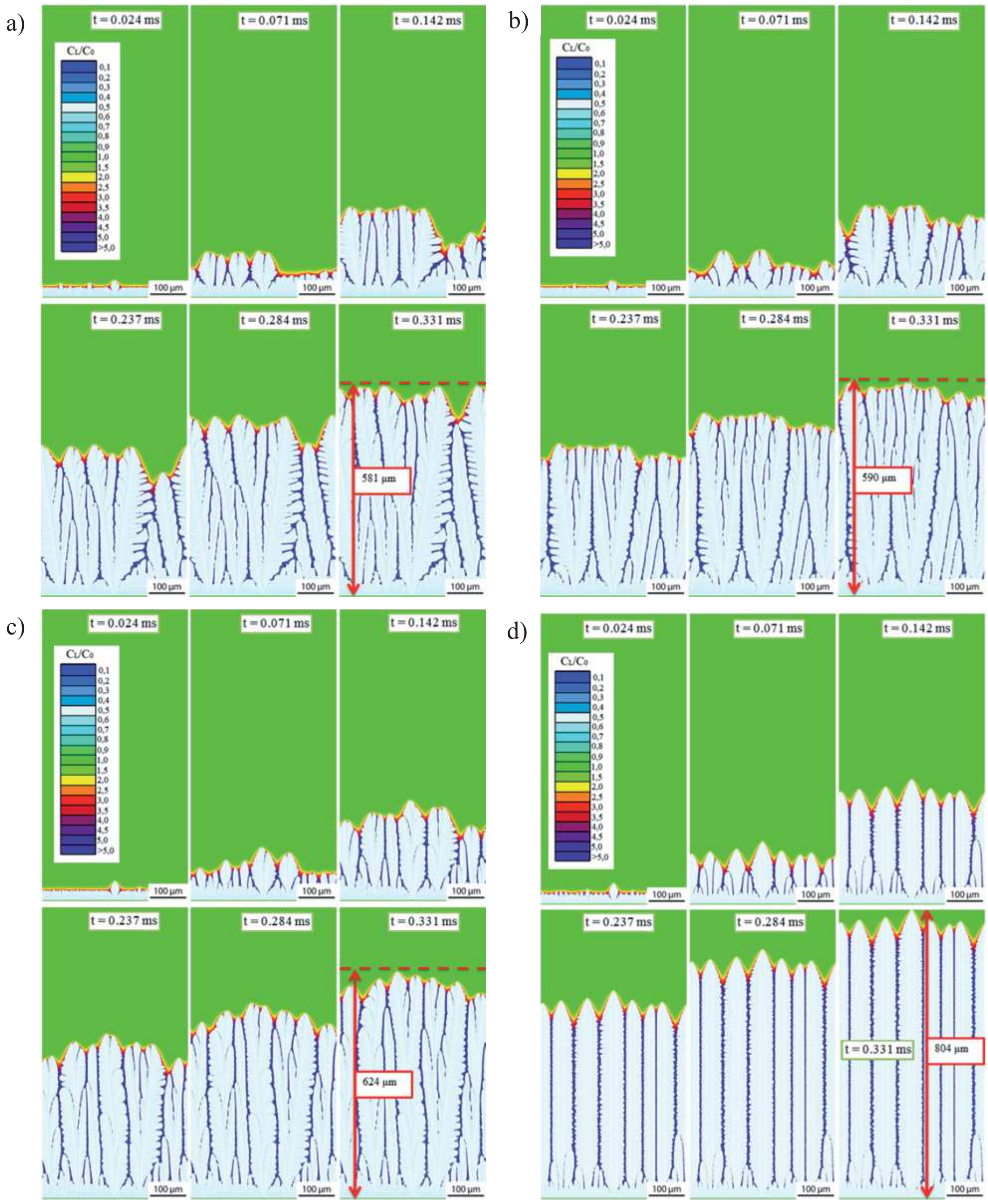

Fig. 3. Evolution of the dendrite structure in time with different density of the inoculants distribution: (a) – φ = 0; (b) – φ = 0.1; (c) – φ = 0.2; (d) – φ = 0.3

Thus, a branched solidification structure with wide branches of dendrites (up to 100 μm) can be observed in absence (Fig. 3a) of the refractory inoculants in the melt metal.

The melt metal with the refractory inoculants, affecting the surface tension between solid and liquid phase, promoted for a change of dendrite structure from branched one to completely columnar morphology (Figs. 3b,c,d). Such a significant change of nature of the metal dendritic structure is only caused by the processes taking place on a contact surface of refractory inoculant with growing dendrite.

In this case TiO_2 is well wetted by the melt that promoted for local solidification rate increase in a contact zone of growing dendrite with inoculant. This occurs due to rise of undercooling in the contact zone (Gibbs-Thompson`s, $\Delta T_G$ effect). Increase of rate of dendrite growth due to Gibbs-Thomson`s effect results in rise of concentration undercooling (ΔT_C) due to pushing out a large amount of the impurity before the solidification front. Also, change of growth rate at the end of dendrite promotes for further deviation of the process from equilibrium and rise of undercooling due to deviation from liquidus equilibrium line (ΔT_N).

Description of nature of development of the physical processes, imbedded in the proposed solidification model, allows simulating quality changes of the weld metal dendrite structure depending on number and properties of the added inoculants. If refractory inoculants are absent, the solidification front in the weld pool moves for 581 mm during 0.331 ms (Fig. 3a), and at their distribution with φ = 0.3 probability this makes 802 mm (Fig. 3c) all other things being equal (including initial solidification rate).

It is necessary to note significant change of the dendrite structure morphology from much branched, formed because of competitive growth of separate crystals, to completely columnar structure. Reduction of wetting angle in the local points of contact of growing dendrite with the metal melt can provide significant qualitative change of the dendrite structure, that, in turn effect further solid phase transformations in metal and as a result final microstructure and mechanical properties of HSLA steels.

Figure 4 presents dimensions' comparison of the dendrite structure, received in computational and experimental way [2,12] for the specimens of the first and second series. An average error of data, obtained by means of computational experiment, makes around 25% and increases with rise of wetting angle of the refractory inoculant by weld pool metal. Such a difference in received results can be related with selection of parameters of distribution of the refractory inoculants in the melt φ equal 0.3. It apparently does not correspond to the conditions of carried experiment researches. This factor should be taken into account in further investigations and it is necessary to study in more details the effect of distribution parameter on development of the weld metal primary structure. Also, the error was introduced by inaccurate composition and model limitations.

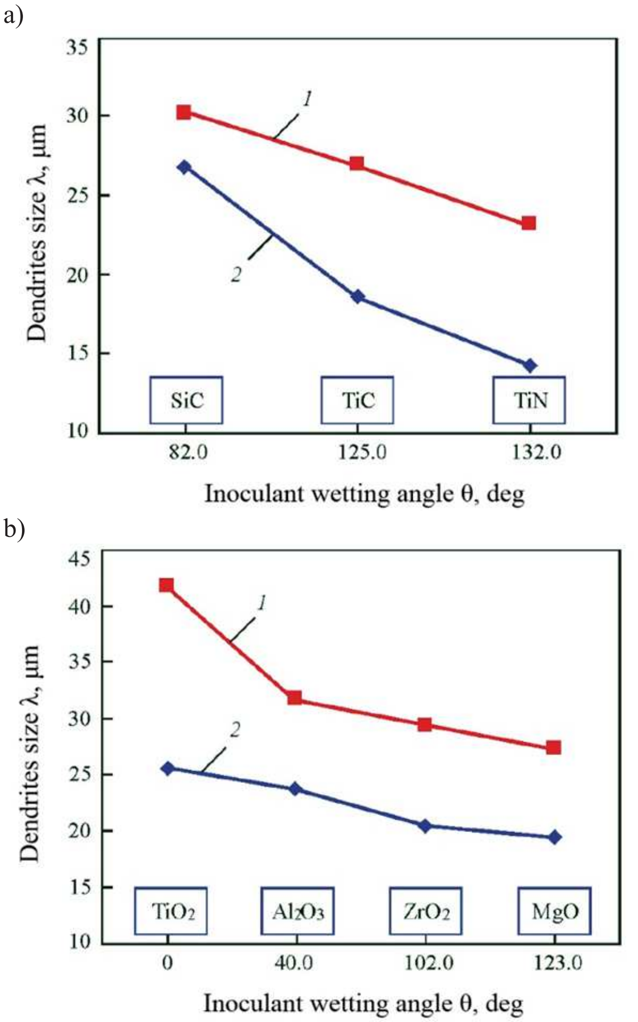

Fig. 4. Comparison of experimental results of measurement and computational data of metal dendrite structure parameters of specimens in the first (a) and second (b) series of experiments: 1 – experimental; 2 – computational

7. Conclusions

The model, based on finite element method coupled with cellular automation method, well suits simulation of solidification process of the HSLA steels melt metal taking into account the refractory inoculants effect on the solidification process. It is related with the fact that the main model of solidification structure development can be easily completed by additional rules and laws of interaction of moving solidification front with inclusions introduced in the melt metal. Also, an advantage of such approach is the possibility of tracing of any parameters of cellular automation discrete cells (concentration of additive, undercooling, coefficient of surface curvature etc.) in time.

Computational experiments, carried by developed software, showed the possibility of influence on parameters and morphology of metal primary structure. Developed model and software, are good for prediction of dimensional parameters and morphology of metal primary structure considering influence of refractory inoculants.

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