Computational Materials Science 108 (2015) 168–176

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

A solution to the problem of the mesh anisotropy in cellular automata simulations of grain growth

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ARTICLE INFO

Article history:
Received 19 December 2014
Received in revised form 15 June 2015
Accepted 16 June 2015
Available online 6 July 2015

Keywords:
Grain growth
Solidification
Mesh anisotropy
Cellular automata

ABSTRACT

Cellular automata modeling is a powerful tool used for simulating complex grain growth phenomena. However, a computational mesh may give rise to artificial anisotropy, which is a highly undesirable calculational problem. To eliminate this drawback of the approach, we have introduced two new corrections into a two-dimensional cellular automata algorithm for grain growth. The two-dimensional cellular automata model built in the framework of the approach developed by Rappaz and Gandin is based on a combination of the cellular automata and finite difference methods. The simulation results obtained for the cases of single grain growth and evolution of polycrystalline structure during solidification of alloys have demonstrated that the proposed corrections enable the mesh anisotropy problem to be solved.

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1. Introduction

Grain structure formed during solidification of alloys produces a profound effect on the attainable mechanical and functional properties of materials and plays a key role in the prediction of their thermomechanical response to different production processes, like casting, welding, or additive manufacturing. This is why an understanding of the microstructural evolution during solidification is important for product design. While the development of experimental techniques facilitates a detailed characterization of solidification microstructures, it is numerical simulations which provide a possibility of deriving the dynamic evolution of grain morphology. With a rapid advance of computer technologies and numerical solution techniques, the simulation of solidification of alloys has become an efficient tool of modern metallurgy studies and enables a large number of factors involved to be examined.

A comprehensive bibliography of the publications relevant to the subject under study is provided in the work of Boettinger et al. [1], with special emphasis being placed on numerical techniques. Some of the most popular tools for simulating grain structures formed during solidification are phase field and cellular automata (CA) methods described in the works of Steinbach et al. [2] and Rappaz and Gandin [3], respectively. Both of the above-mentioned approaches provide precise reproduction of the features inherent in the microstructural evolution during solidification of alloys. A detailed description of the phase field method can be found elsewhere (see, for example, [2]). It should be noted that while the phase field method is relatively straightforward to implement, it takes considerable computing power, and the dendrite growth simulation is limited to a small region containing only a few grains [4]. This work focuses on the CA method for simulating complex grain morphologies, taking into account the nucleation and growth of solidification grains. This approach has originated from the pioneering work of Rappaz and Gandin [3]. The model has evolved into a CA model coupled with finite element (CAFE) [5], finite difference (CAFD) [6,7], finite volume methods (CAFV) [8], and the like. The CA models have been used for simulating the processes operating at the meso- (see, for example, [3,5]) and microscale levels (see, for instance, [9,10]). The mesoscale level describes the microstructural features inherent in the grains of the material, i.e. grain growth is simulated. The microscale level enables complex grain morphology to be described. In other words, it is the dendrite growth which is simulated here.

The CA-based simulation is not problem-free. Artificial anisotropy is caused by CA square meshes. Grains lose their initial orientations and are aligned with or set at an angle of 45° to the global axis. Numerous investigations have been performed to eliminate the loss of the initial grain orientation. Anderson et al. [11] and

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http://dx.doi.org/10.1016/j.commatsci.2015.06.026
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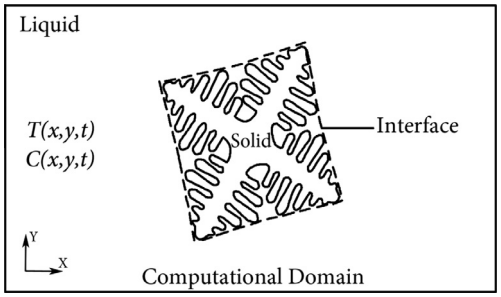

Fig. 1. Schematic of the computational domain in a 2D solidification problem.

Spittle and Brown [12] were faced with a similar problem, using a Monte Carlo grain growth algorithm. They tried to remedy the situation by means of hexagonal meshes rather than of square ones. Rappaz and Gandin [3] proposed "a dendrite tip correction" to be solely applied at uniform temperatures. For this reason, a new procedure was developed by Gandin and Rappaz [13]: a "two-dimensional (2D) rectangular algorithm", as it was called. This technique can be used for any temperature field, but it is difficult to extend it to the 3D case. That is why Gandin and Rappaz [5] built a "decentred square algorithm" which likewise was too complicated to execute.

As regards the mesoscale grain growth, there are a few variants or modifications of the CA models for reducing artificial mesh anisotropy. For the most part, the modeling efforts were concentrated on dendrite growth simulations (see, for example, review [14]). The currently available mesh anisotropy reduction methods for dendrite growth not all are applicable to mesoscale grain growth simulations. It is worth noting that the dendrite growth models and their modifications developed to reduce the artificial anisotropy require sufficiently high mesh resolution.

To solve the artificial mesh anisotropy problem, Marek [15] worked out a new method called GARED that includes additional diffusion to control the grain growth rate. The function introduced to scale the grain interface velocity depends on a numerical parameter φ obtained from a finite difference (FD) solution of the diffusion equation and defined at a point. Thus, the computational domain is characterized by so-called pilot field $\varphi_{i,j}$ which is considered to be "a smeared-out version" of the cell state field. The resulting model demonstrates the capability of the method to simulate the anisotropic growth with a reduced mesh effect. An important issue is that a successful reduction of the mesh anisotropy is attained without introducing any variations into cell capture rules or front tracking. Since the results [15] were obtained using fairly high resolution meshes, only early dendrite growth stages were discussed, and only single dendrite growth was simulated.

Dealing with microscale grain growth simulations, Beltran-Sanchez and Stefanescu [16] built a CA model wherein a solution of the mesh anisotropy problem was suggested. The model minimizes the artificial anisotropy by extending the arc length of the solid–liquid interface to more than one cell. The method allows for simulation of dendrites growing in any preferred direction. The dendrite growth parameters obtained with the use of the model (for example, secondary dendrite arm spacing, tip liquid concentration, etc.) were compared with experimental data or classical Lipton–Glicksman–Kurz (LGK) analytical theory. However, while early in the dendrite growth the initial preferred orientation is retained, it changes with time. Reuther and Rettenmayr [14] believe that with the approach developed by Beltran-Sanchez and Stefanescu, the mesh anisotropy does affect the dendrite growth pattern.

Zhan et al. [17] worked out a limited angle method. They used multi-layer meshes to simulate the grain growth with stochastic orientations. The method is quite simple to implement, its efficiency is illustrated using single and multiple dendrite growth with different orientations as examples. A disadvantage of the approach is that the simulations are time consuming because of the multi-layer mesh. A tracking neighborhood method was proposed by Zhao et al. [18]. Following the approach, the centers of the nearest neighbors of the ith cell (nucleus) are considered to potentially belong to the ith grain depending on the grain growth orientation. Due to the random grain orientation, the centers of the neighboring cells deviate from their original positions.

The present work is devoted to a 2D CA model based on the method developed by Rappaz and Gandin [3] but modified in such a way as to reduce the mesh anisotropy. The model is used to simulate single grain growth and formation of polycrystalline structure during solidification of alloys.

2. Formulation of the model and the features of the numerical solution

Solidification of alloys in a 2D rectangular domain with an interface between the liquid and the solid phases is represented schematically in Fig. 1. The computational domain is initially characterized by a uniform temperature T_0 and a uniform composition C_0. The solidification is initiated when the metal temperature T is below the liquidus temperature T_L, and grain nucleation and growth govern the formation of grain structure. According to Rappaz and Gandin [3], the final grain structure of the material obtained in a number of industrial processes, such as welding, casting, etc., can be adequately described with allowance made for (i) heterogeneous grain nucleation on the surface and in the bulk of the melt, (ii) grain growth with preferred orientations which are generally of the $\langle 1\,0\,0\rangle$ type for cubic metals, and (iii) grain growth kinetics determined with the use of the model suggested by Kurz et al. [19]. The shape of dendritic crystals can be approximated by the cubic form (square form in the case of 2D simulations).

2.1. Heat transfer

The governing equation is of the form:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T), \tag{1}$$

where ρ is the density, c_p is the specific heat capacity, and λ is the thermal conductivity.

Boundary conditions of several types can be applied at the walls of the computational domain [20]. In this work, use is made for the most part of the boundary conditions of the third type. Here the convective heat transfer coefficients κ_l and κ_r for the left- and right-hand boundaries are known and we get

$$\begin{aligned} x = 0 &: -\lambda \tfrac{\partial T}{\partial x} = \kappa_l (T^{e_l} - T), \quad t > 0, \kappa_l > 0 \\ x = N_x &: -\lambda \tfrac{\partial T}{\partial x} = \kappa_r (T^{e_r} - T), \quad t > 0, \kappa_r > 0 \end{aligned}, \tag{2}$$

where T^{e_l} and T^{e_r} are the environmental temperatures at the left- and right-hand boundaries, respectively. The boundary conditions are formulated in a similar way for the top and bottom boundaries, with κ_t and κ_b being the convective heat transfer coefficients. To solve the heat transfer Eq. (1), use is made of an implicit FD scheme [20] which provides the first- and second-order accuracy in time and space, respectively, and is unconditionally stable. Eq. (1) is discretized using a locally one-dimensional unconditionally stable scheme developed by Samarskii [21,22].

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