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Stochastic simulation of grain growth during continuous casting

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Abstract

The evolution of microstructure is a very important topic in material science engineering because the solidification conditions of steel billets during continuous casting process affect directly the properties of the final products. In this paper a mathematical model is described in order to simulate the dendritic growth using data of real casting operations; here a combination of deterministic and stochastic methods was used as a function of the solidification time of every node in order to create a reconstruction about the morphology of cast structures.

Keywords: Continuous casting; Dendrite; Mathematical simulation; Chill; Columnar and equiaxed zones

1. Introduction

The final quality and properties of castings products depends on the microstructure formed during solidification. The simulation on grain scale is used to provide a reliable foundation for the process control and the improvement of the casting products so, that many authors have been developing mathematical models, algorithms and simulation systems to predict it [1–20].

In the 1960s Oldfield [1] was one of the beginners who tried to simulate the solidification structure. In the 1980s, the Monte Carlo method was used for modeling the nucleation and growth of the grains. In the early 1990s, cellular automaton model was employed in which the physical mechanism of heterogeneous nucleation and growth was taken into account and in a similar way deterministic methods were introduced to deal with the distribution of the nuclei. In recent years, the phase-field model has been developed to simulate the formation of microstructures [2,3].

In general, there are two basic theoretical approaches to describe the grain growth: deterministic and stochastic, the others ways are combination of these two. In deterministic methods, the behavior of each grain is determined by established parameters like size, number of neighboring grains and others, while the stochastic methods were first used by Louat and then modified by some other authors [4–7].

Deterministic approach refers explicitly to the driving force of grain growth, which is due to the decrease in total grain boundary energy. Nevertheless, this approach is standard but leads to wrong predictions of the grain size distribution. Therefore it is necessary to increase the state parameters and obtain better results. On the other hand, the stochastic approach is much more successful in predicting size distributions because this approach can reproduce the heterogeneity of materials using random grain sizes and populations.

A very important problem involved in grain growth simulation is that the number of cells needed to simulate the microstructure of a casting is tremendous due to the scale of the grain size. Consequently, the efficiency of a personal computer will be very low, the reason why some authors have explored using parallel computing techniques [3]. Nevertheless, improving the algorithms to simulate accurately the phenomenon is other possible way. It is important to remember that the number of cells is a function of the scale used to simulate the micro- or macro-scale phenomena, and very large array sizes require longer times to analyze and create a good approach.

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Nomenclature

a_1	chill zone size (mm)
a_2	columnar zone size (mm)
a_3	equiaxed zone size (mm)
d_1–d_4	distances from the pivoting node to billet surfaces (mm)
n_R	random number
t	simulation time (s)
t_a	time defining if a node is nucleated or growth
t_1	time defining limit of chill zone (s)
t_2	time defining limit of the columnar zone (s)
$t_{I,J}$	pivoting node
$t_{liq,I,J}$	time for which liquid state of the pivoting node exists (s)
$t_{mushy,I,J}$	time for which mushy state of the pivoting node exists (s)
$t_{sol,I,J}$	final point of solidification of the pivoting node (s)
$t_{x,y}$	neighbor of the pivoting node
$X_{sol,I,J}$	solid fraction in pivoting node (%)
x,y	positions of the neighbors of the pivoting node

2. Nucleation and growth model

The first step to develop a model to describe the grain growth process is to understand the phenomena physically involved in it.

When a liquid metal is quenched, the nucleation and growth process will appear. The atoms in the domain are moving in liquid conditions, but they form clusters as their temperature decreases below liquidus. When the cluster grows to a certain size it becomes a crystalline nucleus, and this process is called nucleation.

When a nucleation point has been established, one or more of the nearest neighbors may tend to join with it; this process is called grain growth.

The solidification grain structure of a cross-section of an ingot shown in Fig. 1. It was described by Flemings [8]. Here three different zones can be identified, one of them is the outer zone also called chill zone, it comprises of fine grains with random orientation. The second, an intermediate zone is a columnar zone, with many elongated and oriented grains from the billet surfaces to the centre. Finally, there is a central equiaxed zone comprising of less randomly oriented grains. Steel solidification during continuous casting is dendritic. Each grain contains one dendrite with a main arm and many secondary arms.

Feng et al. [3] and Lan et al. [9] used a cellular automaton model to describe the microstructure of some alloys based on a very similar equation for drawing the profile of a dendrite. To predict its evolution in a micro-scale they used Eqs. (1) and (2) to describe the geometry adopted by the nucleated points, where θ and β are the polar angles of the dendrite, $a = 1.25$ a constant and L and η are the average dendrite radii. These authors show the evolution of the dendrite shape in a liquid pool;

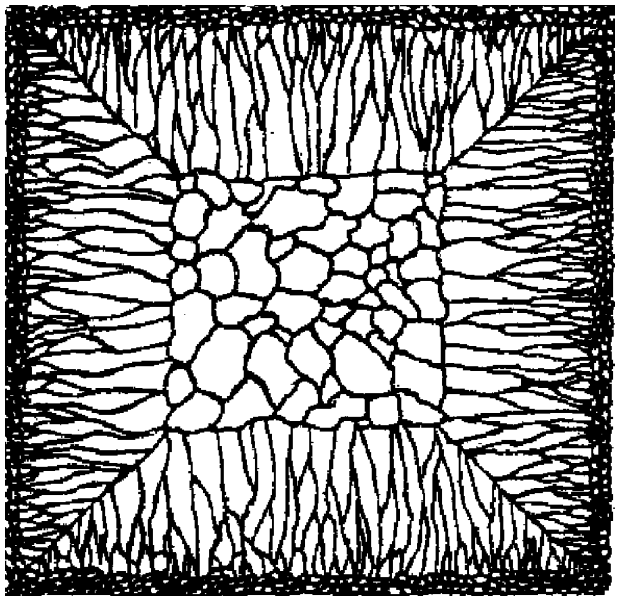

Fig. 1. Sketch of ingot grain structure showing chill, columnar and equiaxed zones [1].

after nucleation, the dendrite was considered to grow along four directions (branches at 90°) and finally tend to adopt a square shape. The result is a group of randomly oriented grains that grow until their borders make contact.

$$L(\theta) = L_0[1 + (a - 1)\cos 4\theta] \quad (1)$$

$$\eta = 1 + \gamma \cos 4\beta \quad (2)$$

Other authors have been developing models to create one in combination with some phenomena like recrystallization [7,10–12], but a very important point is the necessity for programming a micro-scale model without losing the macro-scale viewpoint. In recent years, many models have been developed [13–20] to simulate grain growth but no one has joined the calculation of a thermal behavior and the solidification times as a base to build a probable structure of the cast products using real operating conditions.

3. Mathematical model

The mathematical model used solves the equations for heat transfer involved during the continuous casting process; firstly, the steel is discretizated using a regular square grid that represents volumes of liquid steel. Heat removal is calculated according to the mechanism of the steel position along the cast machine.

For the billet surface different border conditions were defined to calculate heat removal.

In the mold, heat removal is calculated using Eq. (3)

$$q = A_0 + B_0\sqrt{t} \quad (3)$$

where the values for the coefficients A_0 and B_0 are 2680 and 335, respectively, as obtained by Savage and Pritchard [21].