Journal of Alloys and Compounds 762 (2018) 508–519

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

A method based on the centroid of segregation points: A Voronoi polygon application to solidification of alloys

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A R T I C L E I N F O

Article history:
Received 11 February 2018
Received in revised form
3 May 2018
Accepted 13 May 2018
Available online 16 May 2018

Keywords:
Segregation
Solidification
Structure
Voronoi polygon
Fractal dimension
Alloy

A B S T R A C T

A new method for controlling segregation delicately based on the centroid of independent segregation points in an alloy macrostructure is established using Voronoi polygon method. Voronoi polygon area is found to nearly obey the log-normal distribution, which shows that a polygon may reflect a new solidifying unit. The relationship between Voronoi polygon characteristics and carbon segregation extent (segregation ratio) is investigated at different locations. In a pure columnar grain zone, the segregation extent worsens as the Voronoi polygon size decreases; in an equiaxed grain zone, this extent worsens as the size increases. A near-equilibrium solidification model for polygons under different conditions is studied, and the results are consistent with the aforementioned finding of segregation ratio. Compared with a secondary arm spacing, the fractal dimension of the solidification structure may be a better method to describe the characteristics of the solidification structure and the size change of Voronoi polygons as to relevant segregation. Thus, this study proposes a new experimental method that depicts the macrostructure from a different perspective, i.e., the segregation point instead of the solidification structure. The formation of Voronoi polygons created by segregation points during solidifying should be divided into two stages, i.e., appearance of the segregation point and determination of the polygon's outline. The segregation extent can be controlled by altering the size of the relevant Voronoi polygon, which is a unique alternative strategy for improving the uniformity of element distribution rather than simultaneously considering nucleus formation, solidification structure growth, and liquid flow as to the complex process of segregation formation.

1. Introduction

Segregation occurs in many metal materials, including alloys. In most multi-component alloys, elements with low distribution coefficients easily segregate during solidification [1]. Element segregation is a vital defect in many processes, such as mold casting and continuous casting [2,3]. Thus, numerous studies have attempted to improve element evenness through different technologies. For example, in view of the slow solidification rate and shallow liquid zone, electro-slag remelting technology (ESR) is a good method for controlling segregation. However, macro or semi-macro segregation still plays a key role in the ESR billet, especially for high-grade alloy products [4]. Therefore, element segregation during solidification is still a key issue concerning the quality of alloy materials.

Solidification theories serve as a fundamental guideline for altering structural formation and eliminating segregation. According to classic theories, nucleus formation and solid phase growth are the main stages of macrostructure formation, and many remarkable works have been carried out for controlling the solidification structure [5–7]. With regard to element nonuniform distribution, many microsegregation models with different assumptions have been developed by many famous researchers [8], such as Brody and Flemings [1], Clyne and Kurz [9], Voller and Beckermann [10], and so on. The formula for local solute redistribution was first proposed by Flemings et al. [11] to quantitatively describe macrosegregation, and this work has since been followed by Fredriksson [12], Rappaz [13], Beckermann [14], and so on. These solidifying models play a significant role in quality improvement and promote the development of many new technologies. However, these theories have mostly highlighted the solidification structure or initial solid phase rather than the segregation points as the focus or the starting point of research. Following the existing methods, many researchers and engineers have to jointly consider many aspects, e.g., nucleation, growth, and liquid flow, to precisely control the segregation. Additionally, compared to the segregation point, the grain nucleus always appears earlier and stops growing finally when encountering other grains during solidification, so

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https://doi.org/10.1016/j.jallcom.2018.05.160
0925-8388/

different grains are very easy to form a complex interweaving network, especially for dendritic structure in multicomponent alloys. Therefore, a complete grain is always unavailable to determine its boundary in a sample, but a segregation point is easily discriminated by its complete independent boundary [4].

In this article, to investigate the macrostructure from the perspective of the segregation point and improve the uniformity of the element distribution, we propose a new method for controlling segregation delicately based on the centroid of segregation points. First, the Voronoi polygon (VP) method was used to reconstruct the macrostructure on the basis of the different centroids of segregation points. Then, the characteristics of the VPs as well as the relationship between the polygon characteristics and the segregation extent are discussed. Finally, the new method is presented and discussed. This idea was motivated by the author's previous works on the segregation morphology [4,15].

The VP method, which is also called Dirichlet tessellation, originated from Thiessen polygons. This approach provides a means of naturally partitioning space into sub-regions to facilitate spatial data manipulation, modeling of spatial structures, pattern recognition, and locational optimization [16]. As a fundamental data structure of analyzing proximity relation, the VP method is used in many fields for different purposes. For example, in material research, Ghosh and Moorthy developed a microstructure-based Voronoi cell finite element model to overcome difficulties in modeling materials with arbitrary phase dispersions [17–19]; Estrin et al. used this method to analyze the deformation behavior of particle-strengthened alloys [20]; Tippur and Sotomayor studied the elastoplastic compression response of 3D structures generated by Voronoi diagrams [21]; Takaki et al. investigated the characteristics of a primary arm array during the directional solidification of a single-crystal binary alloy through Voronoi decomposition and Delaunay triangulation [22]. However, no study has utilized the VP method to analyze the alloy macrostructure from the perspective of segregation points.

2. VP based on the centroid of segregation points

2.1. Macrostructure and segregation morphology

The selected alloy's main chemical compositions include C (0.38 wt%), Cr (4.98 wt%), Mo (1.33 wt%), V (0.99 wt%), and Fe (92.32 wt%). The related billet is produced by ESR technology. Fig. 1 shows the sampling position, which is perpendicular to the left and right sides (in the casting direction viewed from the top) and across the billet center. A total of 12 samples (#1–#12) are along the centerline of the billet symmetrically, and each sample has a size of 10 mm × 10 mm. Then, these samples are etched with warm 50% hydrochloric acid–water solution to reveal the macrostructure. In this hot pickling experiment, the bath temperature is 60–80 °C, and the etching time is 25 min. These macrostructures are photographed by SELP1650 high digital camera. Given that carbon has the lowest distribution coefficient and is easier to react with hydrochloric acid–water, the macrostructure is composed of the solidification structure (white color part) and positive segregation points of carbon (black color part), as shown in Fig. 2.

Fig. 2 depicts that the solidification structures in the middle zone (samples #5–8, i.e., Fig. 2(e) and (h)) are mainly equiaxed grains, whereas the solidification structures in the outer zone are mainly columnar grains (sample #1–#4 and #9–#12, i.e., Fig. 2(a) and (d) and Fig. 2(i) and (l)), particularly in samples #1 (Fig. 2(a)) and #12 (Fig. 2(l)) which nearly completely comprise pure columnar grains.

The quantitative measurement of the segregation extent from the macrostructure morphology is beneficial to the delicate control

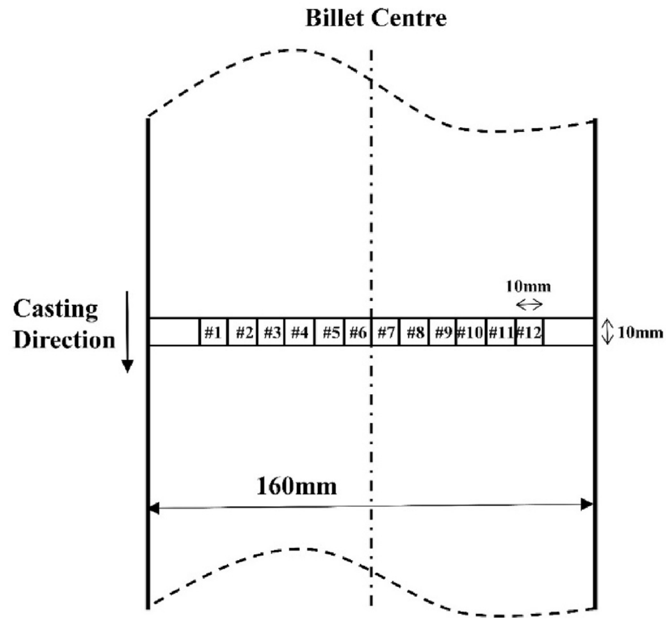

Fig. 1. Schematic of the sampling location in the central plane of the billet [4].

of the segregation. For this purpose, the segregation ratio [4] is introduced and defined in Eq. (1). Given that positive segregation points of carbon are displayed with a black color after the hot pickling experiment, a larger segregation ratio indicates that a sample solidifies with higher segregation extent.

$$R = \frac{A_{seg}}{A_t} \times 100\% \tag{1}$$

where R is the segregation ratio, %; A_{seg} is the area of segregation points (black part), mm^2; A_t is the total analyzing area, mm^2.

For each sample in Fig. 2, the value of A_t is 10 mm^2, and the corresponding R is called as R_w (whole segregation ratio). Because the sampling location in the central plane of the billet is perpendicular to casting direction and along the main trunk section for columnar grain, the macrostructure in each sample can be representative. Meanwhile, the sample size is 10 mm × 10 mm which is big enough to contain plenty of grains and segregation points. Thus, the segregation ratio based on two dimension section should reflect effectively the segregation extent in three dimension volume. Fig. 3 shows the R_w at different sample numbers. From the outer to the middle zones of the billet, the whole segregation ratio initially increases and subsequently decreases in the equiaxed grain zone. As shown in Fig. 4, the segregation area at different locations is generally composed of one thousand segregation points of different sizes. On the basis of the area, the segregation points can be divided into two types (I and II). The areas of the I- and II-type segregation points are $\geq$0.01 and < 0.01 mm^2, respectively. Comparison of Fig. 5(a) and (b) reveals that the segregation ratios in the billet are mostly influenced by the large segregation point (the area ratios of the I-type segregation exceed 90%), although its amount ratio is about 40%. Therefore, the large segregation points should be mainly considered to alleviate the segregation phenomenon, and I-type segregation points are chosen for creating the VPs.

2.2. VP method

The VP method, which originated from meteorologist Thiessen, is aimed to divide a plane into different polygons that are based on different discrete points. Polygons have three characteristics. First,