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Chord length distribution of Voronoi diagram in Laguerre geometry with lognormal-like volume distribution

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Abstract

The Voronoi diagram in the Laguerre geometry based on random close packing of spheres (RCP-LV diagram) has been found to be a better representation of polycrystalline structure than the conventional Poisson–Voronoi diagram. Stereology of the RCP-LV diagram with lognormal-like volume distribution has been investigated by the classical intercept count method. An improved five-parameter gamma distribution function is proposed to integrate the fact that probability density of the chord length remains non-zero as the chord length approaches zero. The proportional coefficient between the average grain size and the average chord length varies from 1.60 to 1.14 as the coefficient of variation of grain volume increases from 0.4 to 2.2. It is shown that there exists the possibility that not only the average grain size but also the grain size distribution can be estimated if the chord distribution characterization is fully explored with the aid of RCP-LV diagram simulation.

Keywords: Chord length distribution; RCP-LV diagram; Volume distribution; Stereology; Proportionality

1. Introduction

The grain size distribution and average grain size in polycrystalline materials have a significant impact on many properties, such as mechanical strength, electrical conductivity and dielectric constant. The average grain size is often taken as a basic quality control standard in industrial procedures. Since the establishment of a structure–property relationship is an essential topic of materials science, a reliable method to measure grain size distribution and average grain size is of general interest.

Generally speaking, such methods can be divided into two categories. The first of these includes those that measure the shape and volume of individual grains by a serial sectioning method [1–3] or chemically distinguishing metal into separate grains [4]. Obviously, these are time-consuming and expensive. Research reports of this kind are indeed rather rare. The second, which has been adopted more extensively, is stereology [5]. A standard method is the

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so-called intercept count method. Random test lines are placed on statistically representative sections and divided into chords by grain boundaries. The chord lengths obtained yield the mean linear chord length, $\langle L \rangle$, which is assumed to be directly proportional to the three-dimensional spatial grain diameter, $\langle D \rangle$ (average value of equivalent spherical radius of grains):

$$\langle D \rangle = k \langle L \rangle \quad (1)$$

Thus, the problem arises that the determination of k, the proportional coefficient, is not straightforward [6]. It depends on the shape distribution and spatial diameter distribution of the grains [7]. The two distributions may or may not be independent. Rhines and Patterson reported that the coefficient of variation (standard deviation divided by mean) of grain volumes (CV_g) ranged from 1.09 to 2.13 in different recrystallized aluminum samples [4]. Thorvaldsen proposed that there was no general proportionality between the mean linear intercept length and the mean spatial grain size, because two samples with equal mean linear chord length might differ in spatial grain diameters by a factor of 2.5, if the possible influence of shape distribution is ignored [7]. Mendelson recommended the use of a proportional constant of 1.56 unless more representative data are available for materials with specific processing conditions [6]. Most research papers published since then have assumed this value of the constant.

Although stereology is powerful and easy for practical application, it has an intrinsic weakness. When a three-dimensional microstructure is sampled on two-dimensional sections or one-dimensional chords, much information is lost. As a result, it is rather difficult to recover the spatial grain size distribution from intercept lengths.

In this paper, we attempt to combine the two classes of methods mentioned above in our computer simulation. The methodology behind it is that the possibility of establishing a more detailed relationship between stereology information and spatial microstructure might be created if enough spatial and stereological data are cumulated simultaneously from a serial of samples. This relationship could be utilized later to estimate the spatial structure property of real materials from its stereological measurement, e.g. chords.

We describe briefly, in Section 2, polycrystalline structures represented as a kind of weighted Voronoi diagram with lognormal-like grain volume distribution. Intercept length distribution is analyzed in Section 3 and correlated to spatial distribution to deduce the specific proportional coefficient k for different microstructures. Potential application of our result is also discussed. Conclusions are drawn in Section 4.

2. Simulation procedure

2.1. RCP-LV diagram (Voronoi diagram in the Laguerre geometry based on random close packing of spheres)

A polycrystalline structure is composed of numerous grains. Several types of models have been used to simulate it, among which the Poisson–Voronoi diagram (PV diagram) has been extensively studied and utilized [8–12]. The PV diagram is assembled with an array of polyhedrons that connect themselves in a topologic manner observed in real materials and which can be treated as grains. However, some inadequate features of the PV diagram do exist in the representation of polycrystalline materials [13,14]. The coefficient of variation of grain volumes (CV_g), for example, is 0.424, obviously lower than those of real materials.

In a previous paper by our group, another type of diagram was proposed as a microstructure model, the RCP-LV diagram [13]. To construct a RCP-LV diagram in a computer model, spheres with specified volume distribution type and distribution parameters (e.g., expectation and variance) are packed randomly and closely [15]. A weighted Voronoi diagram, i.e., an RCP-LV diagram, is then imposed on this sphere configuration. In the RCP-LV diagram, each sphere has its own polyhedron, which, in turn, encloses the whole sphere. Thus, the volume distribution of the polyhedron inherits strongly that of the original spheres. Both the volume distribution shape (measured by the probability density function, pdf) and the corresponding CV value (CV_g) can thus be controlled to some extent in a microstructure simulation procedure. A lognormal-like distribution results when the volume distribution of spheres is lognormal and its CV_g can be varied systematically [13]. We have