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On the determination of grain-size distributions from intercept distributions

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A matrix formulation for determining the spatial grain-size distribution of tetrakaidecahedral grains from linear-intercept data is developed. The truncation effect (which stems from the fact that the intersection of single-size grains by a test line gives rise to intercepts of different length) and the sampling effect (which results as a consequence of bigger grains being intersected more frequently than smaller ones) are separately taken into account. The derivation procedure of this formulation is applicable to any other convex shape, provided the linear intercept distribution for single-size grains of the corresponding shape is known. The percentage spatial grain-size distributions obtained by the formulation derived here are similar to those estimated by the Spektor's chord method for spherical grains.

1. Introduction

The main difficulty found in grain and particle size distribution analysis from opaque samples arises from the virtual impossibility of directly measuring the true-size distribution. A useful procedure of providing the experimental data required to calculate the spatial size distribution, makes use of the distribution of intercepts of a test line with grains [1]. Moreover, it is well established that the spatial size distribution differs from the intercept length distribution because of the truncation and sampling effects [1]. The former effect stems from the fact that the intersection of single-size grains by a test line gives rise to intercepts of different length, while the latter results as a consequence of bigger grains being intersected more frequently than smaller ones.

Several methods for computing true-size distributions from linear analysis have been developed, particularly for spherical and ellipsoidal geometries [1–3]. Another reasonable choice for the grain shape is a tetrakaidecahedron (truncated octahedron). In fact, a distribution of complex polyhedra exists; however, a tetrakaidecahedral shape is of interest since it corresponds to the plane-faced polyhedron which, for single-size grains, best satisfies the minimum surface-energy and space-filling requirements [4–6]. This shape has been previously assumed [7–12]. Attempts have been made to obtain the spatial grain-size distributions for tetrakaidecahedral grains from linear intercepts [11, 12]. These attempts, however, have actually only considered the truncation effect.

In this work, a matrix method for the determination of spatial grain-size distributions of tetrakaidecahedral grains from linear intercept distributions is developed. The present method, which separately takes into account the two above effects, is mainly based on two previously reported works [3, 12]. Some conclusions inferred from the application of this method are also presented.

2. Method formulation

2.1. Foundations of the method and the truncation effect

As a result of the truncation effect, the distribution of linear intercept measurements of a set of grains will range from zero to a maximum value, even for single-size grains [1]. In fact, the distribution of intercepts for single-size

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TABLE I Distribution of linear intercepts for single-size tetrakaidecahedral grains [11]

	Class number							
	8	7	6	5	4	3	2	1
Range (l/l_{max})	0–0.13	0.13–0.18	0.18–0.24	0.24–0.30*	0.30*–0.42	0.42–0.56	0.56–0.75	0.75–1.00
Relative frequency†	0.013	0.005	0.026	0.047	0.083	0.176	0.295	0.365

*We think that this value should be changed to 0.32.
†Note that the sum of these eight original relative frequencies yields 1.010.

tetrakaidecahedral grains has been previously determined [11]. In that work, the distribution of intercepts was divided into eight classes, adopting a geometric scale of module 4/3. The upper limit of this distribution is the value of the maximum intercept length, l_{max}, corresponding to the size of the pertinent tetrakaidecahedral body. The fractional frequencies associated with each of these classes [11] are reproduced in Table I. In the following, these classes will be referred to by the indices i (i = 1 to 8) as indicated in Table I. Also, the upper limit of class i will be denoted by l_i (i = 1 to 8).

Table I can be directly employed for establishing the spatial grain-size distribution of non-single-size tetrakaidecahedral grains intersected by a test line. The purpose of this section, where only the truncation effect is considered, is the determination of such a distribution. The matrix formulation for accomplishing this purpose, presented below, is a rederivation of the procedure previously proposed by Haroun [12]. The rather extensive derivation that follows is necessary to clearly overcome some defects of the original formulation.

For determining the spatial size distribution of intersected grains, the experimental distribution of intercepts is divided into the same classes as shown in Table I. Note that, in such a case, the upper limit of the intercept distribution is, in principle, equal to the maximum observed intercept length, L. Moreover, the spatial grain-size distribution is approximated by a discrete distribution of eight grain sizes, D_i (i = 1 to 8). The spatial sizes are defined so that the maximum intercept length corresponding to grain size D_i, coincides with the upper limit, l_i, of intercept class i. (The intercept class and grain size definitions stated above are consistent with those of Haroun's work [12].) It must be remarked that indices i (i = 1 to 8) are now employed to refer to classes corresponding to the actual distribution of intercepts.

Thus, if N_1 grains of size D_1 were intersected, then, according to Table I, they would cause 0.365 N_1 intercepts of class 1, 0.295 N_1 intercepts of class 2, 0.176 N_1 intercepts of class 3, . . . 0.005 N_1 intercepts of class 7 and 0.013 N_1 intercepts of class 8. Similarly, if N_2 grains of size D_2 were intersected, they would generate 0.365 N_2 intercepts of class 2, 0.295 N_2 intercepts of class 3, 0.176 N_2 intercepts of class 4, . . . 0.026 N_2 intercepts of class 7, and attention! (0.005 + 0.013) N_2 intercepts now fitting class 8. Analogously, if N_3 grains of size D_3 were intersected, they would cause 0.365 N_3 intercepts of class 3, 0.295 N_3 intercepts of class 4, 0.176 N_3 intercepts of class 5, . . . 0.047 N_3 intercepts of class 7 and (0.026 + 0.005 + 0.013) N_3 intercepts fitting class 8. The intercept contributions of grain sizes D_4, D_5, D_6, D_7 and D_8 can also be derived in a similar way; only the contributions of grain sizes D_7 and D_8 will now be calculated. So, if N_7 grains of size D_7 were intersected, they would cause 0.365 N_7 intercepts of class 7 and (0.295 + 0.176 + 0.083 + 0.047 + 0.026 + 0.005 + 0.013) N_7 intercepts fitting class 8. Finally, if N_8 grains of size D_8 were intersected, they would cause (0.365 + 0.295 + 0.176 + 0.083 + 0.047 + 0.026 + 0.005 + 0.013) N_8 intercepts of class 8; this sum gives 1.010 N_8 intercepts. Note that grains of the smallest size D_8 contribute with intercepts only to intercept class 8 and, in principle, with exactly N_8 intercepts.

From the above reasoning, it follows that the number of intercepts, n_i, of class i (i = 1 to 8) and the number of intersected grains N_i, of size D_i (i = 1 to 8), can be related by the matrix expression:

$$\mathbf{n} = |\mathbf{B}|\mathbf{N} \tag{1}$$

or

$$\mathbf{N} = |\mathbf{B}|^{-1}\mathbf{n} \tag{2}$$

where $\mathbf{n}$ is the column vector of the number of

TABLE II Coefficients of matrix $|\mathbf{B}|$ in Equation 1

0.365	0	0	0	0	0	0	0
0.295	0.365	0	0	0	0	0	0
0.176	0.295	0.365	0	0	0	0	0
0.083	0.176	0.295	0.365	0	0	0	0
0.047	0.083	0.176	0.295	0.365	0	0	0
0.026	0.047	0.083	0.176	0.295	0.365	0	0
0.005	0.026	0.047	0.083	0.176	0.295	0.365	0
0.013	0.018	0.044	0.091	0.174	0.350	0.645	1.0

intercepts n_i ($i = 1$ to 8), $\mathbf{N}$ is the column vector of the number of intersected grains N_i ($i = 1$ to 8), and $|\mathbf{B}|$ and $|\mathbf{B}|^{-1}$ are the corresponding coefficient matrices. The complete expressions for matrices $|\mathbf{B}|$ and $|\mathbf{B}|^{-1}$ are shown in Tables II and III, respectively. In this way, the vector of the distribution of intersected grains, $\mathbf{N}$, can be obtained from the vector of the intercept distribution, $\mathbf{n}$, simply by pre-multiplication of the latter by the inverse matrix $|\mathbf{B}|^{-1}$ which takes into account the above-mentioned truncation effect.

Haroun [12] originally deduced expressions for matrices $|\mathbf{B}|$ and $|\mathbf{B}|^{-1}$, employing a procedure on which the one developed above is founded. Unfortunately, in that primitive deduction some errors slipped in. Apart from the fact that Haroun's $|\mathbf{B}|$ matrix is rotated by half a turn with respect to its appropriate state (possibly, a clerical error), it appears that the procedure used by Haroun [12] for estimating the contributions of grain sizes D_2, D_3, D_4, D_5, D_6, D_7 and D_8 to the class of the smallest intercepts, here referred to as class 8, was incrorrect. In other words, seven of the eight coefficients of what corresponds to the eighth row vector of the present $|\mathbf{B}|$ matrix, were erroneously calculated by Haroun [12].

Moreover, as only the truncation effect was considered by Haroun [12], the distribution which was actually calculated in his paper, was that of the size of grains intersected by a test line. To obtain the distribution of the number of grains of each size per unit volume, or real grain-size distribution, the sampling effect should also be taken into account [1].

2.2. Sampling effect and final expressions of the method

In the present section, through the consideration of the sampling effect, a final matrix expression is obtained for the calculation of the number of grains of each size D_i ($i = 1$ to 8) per unit volume from the number of intersected grains of each size D_i given by Equation 2.

It has been stated by DeHoff and Bousquet [3] that the average of the projected area of convex randomly oriented grains of size D on a plane perpendicular to the test line, is equal to $k_1 D^2$, where k_1 is a constant shape factor. As a consequence, the number of intersected grains of size D_i by a test line of length S (for convex randomly oriented grains of the same shape), is given by the expression:

$$N_i = k_1 D_i^2 N_i^{\mathrm{v}} S \tag{3}$$

where N_i^{v} is the number of grains of size D_i per unit volume. Here, the grain size, D_i, will be defined as equal to its corresponding maximum intercept length, i.e. $D_i = l_i$. So, since l_1 is equal to L, the value of the maximum actually observed intercept length, the grain size, D_i, is equal to $(3/4)^{i-1} L$ ($i = 1$ to 8). Thus, Equation 3 can be re-written as:

TABLE III Coefficients of matrix $|\mathbf{B}|^{-1}$ in Equation 2

2.740	0	0	0	0	0	0	0
−2.214	2.740	0	0	0	0	0	0
0.469	−2.214	2.740	0	0	0	0	0
0.066	0.469	−2.214	2.740	0	0	0	0
−0.129	0.066	0.469	−2.214	2.740	0	0	0
0.055	−0.129	0.066	0.469	−2.214	2.740	0	0
0.063	0.055	−0.129	0.066	0.469	−2.214	2.740	0
−0.060	0.003	0.059	−0.071	−0.004	0.469	−1.767	1.0

TABLE IV Coefficients of matrix $|\mathbf{A}|$ in Equation 6

2.740	0	0	0	0	0	0	0
−3.936	4.871	0	0	0	0	0	0
1.482	−6.997	8.660	0	0	0	0	0
0.371	2.635	−12.44	15.40	0	0	0	0
−1.289	0.659	4.685	−22.12	27.37	0	0	0
0.977	−2.291	1.172	8.328	−39.32	48.66	0	0
1.989	1.736	−4.072	2.084	14.81	−69.89	86.50	0
−3.367	0.179	3.311	−3.985	−0.224	26.32	−99.17	56.12

$$N_i^{\vee} = \frac{1}{k_1 L^2 S}\left(\frac{4}{3}\right)^{2i-2} N_i \qquad (4)$$

Moreover, the above expression can be stated in matrix form as:

$$\mathbf{N}^{\vee} = \frac{1}{k_1 L^2 S}|\mathbf{C}|\mathbf{N} \qquad (5)$$

where $\mathbf{N}^{\vee}$ is the column vector of the number of grains per unit volume, $\mathbf{N}$ is the column vector of the number of intersected grains and $|\mathbf{C}|$ is a diagonal matrix whose coefficients are given by $C_{ii} = (4/3)^{2i-2}$. Note that the coefficients of the sampling-effect matrix $|\mathbf{C}|$ only depend on the grain-size definitions employed.

From Equations 2 and 5 a direct matrix expression for the vector of the number of grains of each size per unit volume, $\mathbf{N}^{\vee}$, as a function of the vector of the number of intercepts, $\mathbf{n}$, corresponding to the previously defined classes, is found:

$$\mathbf{N}^{\vee} = \frac{1}{k_1 L^2 S}|\mathbf{A}|\mathbf{n} \qquad (6)$$

where $|\mathbf{A}| = |\mathbf{C}|\,|\mathbf{B}|^{-1}$. The coefficients derived in the present case for matrix $|\mathbf{A}|$ are presented in Table IV.

3. Application and discussion

The procedure derived above was applied to a

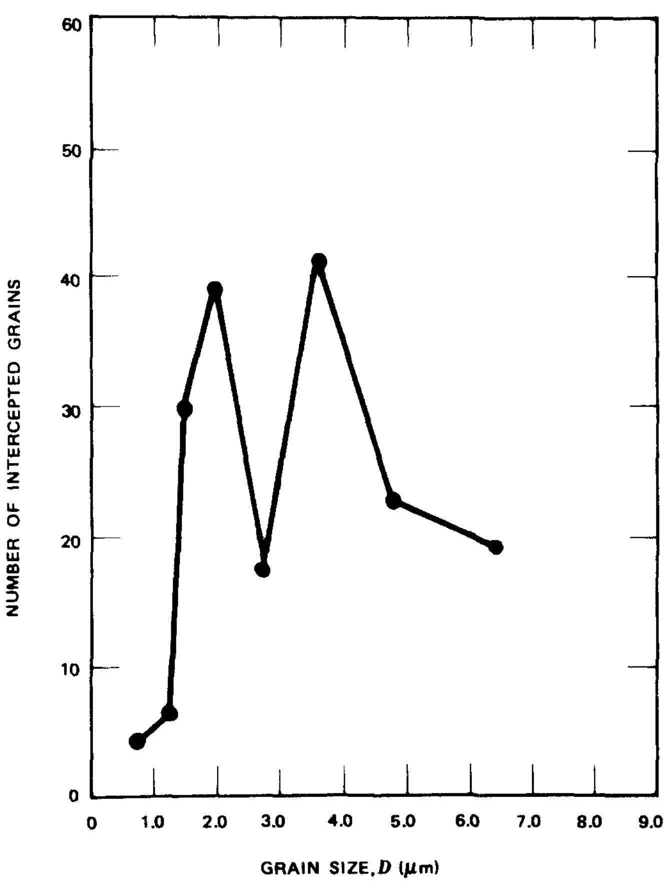

Figure 1 The size distribution of intersected γ_2 particles in a spheroidized Cu–Al eutectoid alloy, derived according to Equation 2.

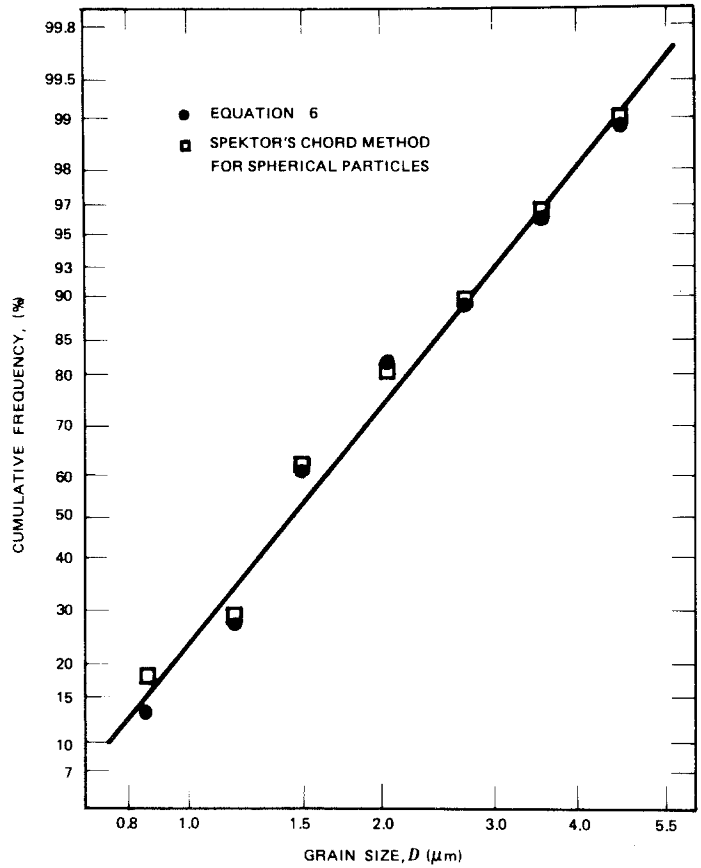

Figure 2 Percentage cumulative frequency against spatial particle-size of γ_2 particles in a spheroidized Cu–Al eutectoid alloy, derived according to the methods indicated.

set of 180 intercept data from γ_2 particles in a spheroidized ($\alpha + \gamma_2$) eutectoid Cu–Al alloy [13]. When only the truncation effect is taken into account, through the application of Equation 2 and Table III (Section 2.1.), the size distribution of intersected particles shown in Fig. 1 is obtained. On the other hand, the spatial particle-size distribution, estimated by means of Equation 6 and Table IV (Section 2.2.) which consider both the truncation and sampling effects, is shown in Fig. 2. In this figure, the results have been represented in a log-probability plot as percentage cumulative frequency of the spatial grain-size distribution as a function of grain size. Percentage frequency and not number of grains was calculated since, to the authors' best knowledge, the value of the corresponding shape factor, k_1, has not been established. Because of the straightness of the plot, this distribution can be identified as being log-normal. Incidentally, the spatial distributions of many alloy systems are closely described by the log-normal distribution [1].

The spatial distribution obtained from the referred γ_2 intercept data by application of Spektor's chord method for spherical particles [2], is also presented in Fig. 2. In this case, the same definition for intercept classes and grain sizes as stated in Section 2.1. were employed. It is seen in Fig. 2 that both computation techniques lead to similar percentage spatial distributions. When the present matrix method and that of Spektor were applied to some other intercept data sets, it was again found that the percentage distributions deduced by both methods were similar, suggesting that this is a fact of ordinary occurrence. This resemblance can be related to the verified similarity between the intercept class frequencies, for the classes defined in Section 2.1., of the intercept distribution for single-size tetrakaidecahedral grains [11], see Table I, and those of the intercept distribution for single-size spherical grains derived by the Spektor's chord method, see Table V.

Finally, notice that the reasoning developed here, where the truncation and sampling effects are separately considered under a matrix form, is a procedure of general validity. Thus, this

TABLE V Distribution of linear intercepts for single-size spherical grains according to Spektor's chord method, for the same intercept classes indicated in Table I

Class number	Relative frequency
8	0.0178
7	0.0139
6	0.0246
5	0.0438
4	0.0779
3	0.1384
2	0.2461
1	0.4375

reasoning can be extended, for establishing spatial distributions from linear distributions, to any other combination of convex grain shape and geometrically scaled intercept classes, provided the distribution of linear intercepts for single-size grains of the corresponding shape is known.

4. Conclusions

A matrix method for determining the spatial grain-size distribution of tetrakaidecahedral grains (or particles) from linear intercepts was derived. The percentage spatial grain-size distributions obtained by this method are similar to those estimated by the Spektor's chord method for spherical grains. The derivation procedure of the present method is extendible to any other convex grain shape, provided the linear intercept distribution for single-size grains of the corresponding shape is known.

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