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The potentialities of a plasticine model of a polycrystal

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A plasticine model of a polycrystal has been constructed with a log-normal distribution of grain sizes. The polycrystal was dissected grain by grain in order to study the topology of the three-dimensional structure. The model was rebuilt with the same grain size distribution and sectioned along various planes. Several parameters of the two-dimensional sections were determined and correlated with the three-dimensional structure. These experiments show the full advantages of this type of model, which have not been exploited previously.

1. Introduction

Most of the detailed descriptions of the topological characteristics of polycrystals have been achieved through the analysis of models obtained by pressing together round particles of a deformable solid to the extent of eliminating all porosity. In this way the particles are transformed into space-filling polyhedral cells connected as the grains in a polycrystal (or the cells in a biological tissue): two polyhedra meet at a face (grain boundary or cell wall), three at an edge and four at a vertex. After pressing, the polyhedra are separated from each other and topologically characterized (number, polygonality and distribution of their faces). A topological analysis of the way the polyhedra are connected is also possible.

There are various examples of studies using models of this type. In the thirties several papers were published by Marvin and by Matzke who used pressed lead shot and examined the resulting grains by means of a dissecting microscope. For example, Marvin [1] used lead shot of uniform size and Matzke [2] made combinations, in various proportions, of two different sizes. In both studies histograms of the frequency of grains with F faces were obtained, the average value $\bar{F}$ of F was calculated and the frequencies of faces with i sides were determined.

More recently, Bernal [3, 4] used plasticine balls of approximately equal sizes instead of lead shot. The balls were rolled in chalk prior to pressing in order to make possible the dissection of the individual grains. The analysis of the polycrystals obtained in this way was not made in detail.

A soap-froth has also been used as a model of a polycrystal. Matzke [5] used this model and described in great detail the topology of individual bubbles, including the distribution and number of faces in each bubble and the polygonality of faces. The paper by Matzke includes a review of the work with the lead shot model and a comparison of the two models with natural biological structures.

The direct topological analysis of a polycrystal can be achieved by the serial section technique, as described by Rhines *et al.* [6]. The method is not easy and is very time consuming, but it allows, at least in principle, a complete topological and geometrical characterization of a polycrystal. Due to its shortcomings the method has never been used to its full potential.

Stereoscopic microradiography is another technique for the analysis of real polycrystals [7, 8], but is of course of limited application. The same can be said about the method based on the fragmentation of a polycrystal upon embrittlement of its grain boundaries [8].

Finally, it should be noted that polycrystals have been simulated in a computer for various purposes (e.g. [9, 10]) but not, as far as we know, to study topological characteristics in detail.

In practice, the information that can be collected on the topology of a polycrystal (and of most biological tissues) is obtained from observations on planar sections of the structure. The interrelation between metric characteristics of the 3-D structure and those of the 2-D sections is, in general, well understood (e.g. [11]) with the notable exception of the lack of an accurate method to find the average grain volume [10]. In contrast, virtually nothing is known about the corresponding correlation between topological properties.

The purpose of this paper is to show the full potentialities of the plasticine model of a polycrystal for studies of various topological problems. In relation to previous work using this and related models, we exploit the possibility of having a pre-chosen distribution of grain sizes and the possibility of making planar sections of the model which can then be analysed in various respects and correlated with the 3-D structure. Examples of various parameters, which were experimentally determined from the plasticine model using a log–normal distribution of grain volumes, will be given for both the 3-D structure and the 2-D sections.

2. The model

A number N of plasticine balls, of different colours to

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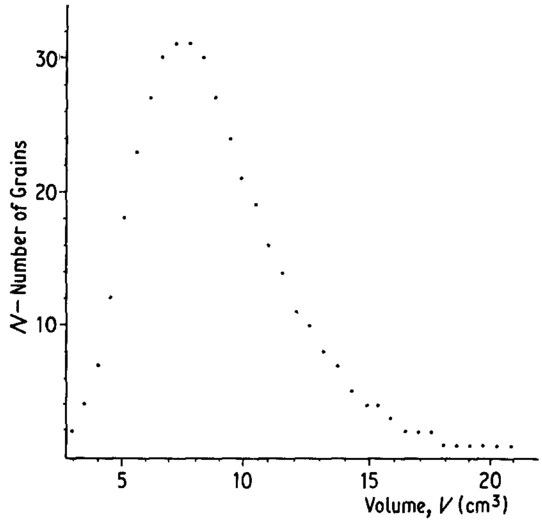

Figure 1 Distribution of grain sizes used in the experiments. The distribution is nominally log-normal; the points were determined by counting the number of grains in classes of amplitude 1 g ($\sim 0.54\,\text{cm}^3$).

facilitate the collection of data, are prepared according to a pre-chosen distribution $n(V)$ of volumes. The volumes V are determined by weighing: $n(V)\,dV$ is the number of balls in the volume interval V, $V + dV$.

Each ball is rolled in common sugar crystals. This is a vital precaution to guarantee the ease of separation of the individual grains after compression. The sugar-covered balls are introduced at random (or otherwise) in a prismatic open mould and compressed into a lump of zero porosity in a press. The polycrystal so obtained can be analysed in two ways, after determining the average volume per grain $\bar{V}$ from N and the direct measurement of the volume (weight) of the lump:

(a) Three-dimensional observations, grain by grain, including the number F of faces per grain, the correlation between F and V, the volume of each grain, the polygonality of the faces and neighbour relations.

(b) Observations on planar sections of the lump, following planes of different orientations. The sections can be analysed to find P_L and P_A (respectively the number of 2-D edge intersections per unit length of random lines and the number of 2-D vertices per unit area of the section), the number of sides i and the area A of the various polygons in the section, and neighbour relations.

3. Experimental procedure

Four hundred plasticine balls (density of plasticine $1.85\,\text{g}\,\text{cm}^{-3}$) was prepared to give a log-normal distribution of grain volumes:

$$n(V;\,\sigma,\,V_0) \;=\; \frac{N}{(2\pi\sigma^2)^{1/2}}\,\frac{1}{V}\exp\left[-\left(\frac{\ln V/V_0}{2^{1/2}\sigma}\right)^2\right] \quad (1)$$

The following values were used: $\sigma = 0.35$; $V_0 = 8.4\,\text{cm}^3$ (15.5 g). Balls in classes of amplitude 1 g were prepared in the range 0 to 50 g, according to the distribution in Equation 1. In each class the weights were random. The experimental distribution curve is shown in Fig. 1. The sugar-covered balls were introduced into a prismatic box (base 160 mm × 160 mm) and pressed to produce a porosity free, approximately cubic, lump. The force used was over 20 kN and the total displacement of the face in contact with the press was approximately 10 cm. The experiment was repeated with the same balls after collecting data on the individual, separated grains. A similar analysis was made for the polycrystal obtained upon the second compression. The planar cuts were made after a third compression of the same distribution and for three orientations of the planes, shown in Fig. 2. Four parallel sections were made for orientations 1 and 3, and five for orientation 2. After each cut, the two halves were stuck together.

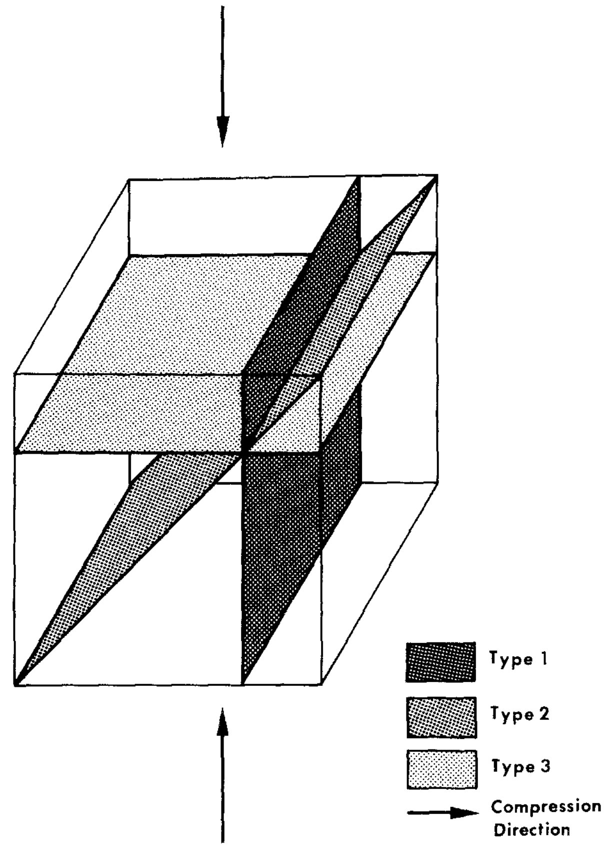

Figure 2 Orientations of planar sections in the plasticine polycrystal used in the determinations of two-dimensional parameters.

The fraction of peripheral grains in the lump was approximately 0.35. These grains and their planar sections were analysed in a special way, by considering that the 3-D or 2-D structure was part of the unit cell (in the crystallographic sense) of a periodic structure. Details of this method will be described elsewhere.

4. Results

4.1. Three-dimensional structure

The faces of the plasticine polyhedra are very well defined but slightly curved, and the number of sides in each can easily be counted. Nevertheless we have not made determinations along this line. All edges have three faces and all vertices have four edges.

The data to be presented are the average of the two experiments using the same distribution. The dispersion of results between the two experiments was found to be small and examples will be given below.

The average volume was $\bar{V} = 8.8\,\text{cm}^3$. The

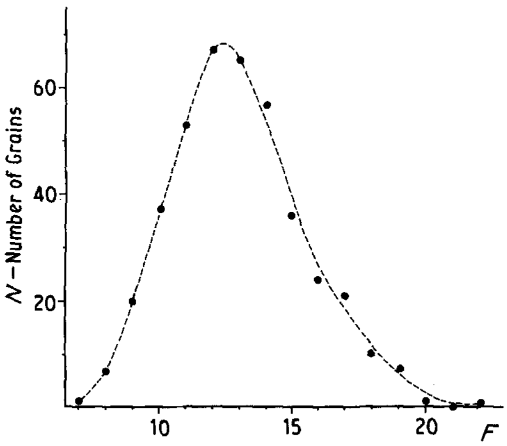

Figure 3 The number of grains as a function of the number of their faces.

distribution of grains according to the number of faces, F, is shown in Fig. 3. The average values $\bar{F}$ obtained in the two experiments were 12.63 and 13.21; we take $\bar{F} = 12.92$. The minimum number of faces found in a grain was 7 and the maximum 22. Fig. 4 gives, for constant F, the number of grains as a function of grain volume V. It is apparent that there is a tendency for large grains to have a larger number of faces. The average volume of grains with a given F is shown as a function of F in Fig. 5. Similar data are shown in Fig. 6, where the average number of faces is plotted as a function of volume. In this figure the results obtained in the two experiments are shown separately. The small dispersion observed (cf. the values of $\bar{F}$ for the two experiments) can be due to a different initial distribution of the balls in the mould. Both plots in Figs. 5 and 6 are nearly linear.

4.2. Two-dimensional sections

Fig. 7 shows a typical section parallel to the compression direction (type 1 section, see Fig. 2). It is apparent that the 2-D edges are curved, reflecting the non-planarity of the grain boundaries.

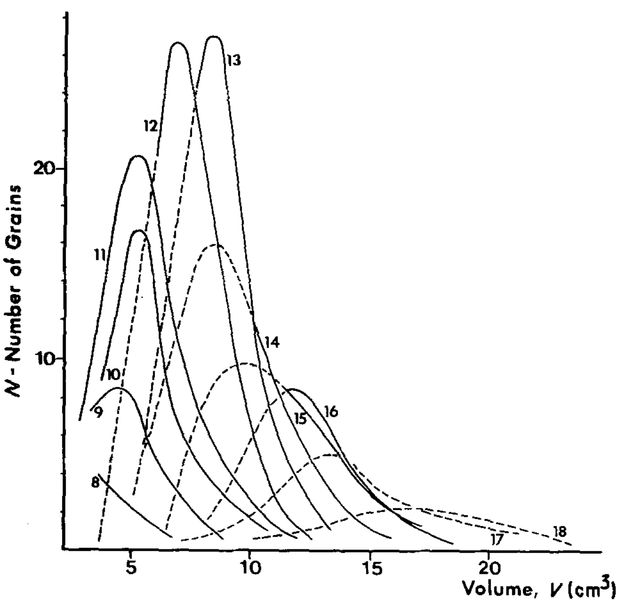

Figure 4 Distribution of grain sizes of constant number of faces, between 8 and 18. Dotted curves are drawn for convenience.

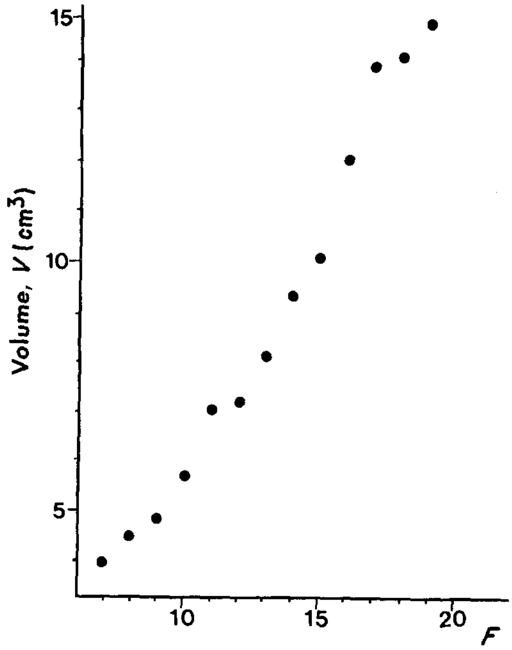

Figure 5 The average volume of grains with the same number of faces, F.

The following results for each type of section are the average for the various sections analysed with the same orientation. In some cases only the average values for all orientations are indicated. The frequency of polygons with i sides is shown in Fig. 8a for each of the three orientations used in the cuts. The average values for all sections are shown in Fig. 8b. Fig. 9 gives the average area of polygons as a function of i. The individual areas were determined by drawing the 2-D network on hard paper, cutting along the edges and weighing. The correlation $A(i)$ is nearly linear. Figs 10a and b show curves for the number of grains as a function of area, for each i and for all polygons, respectively. These can be compared with

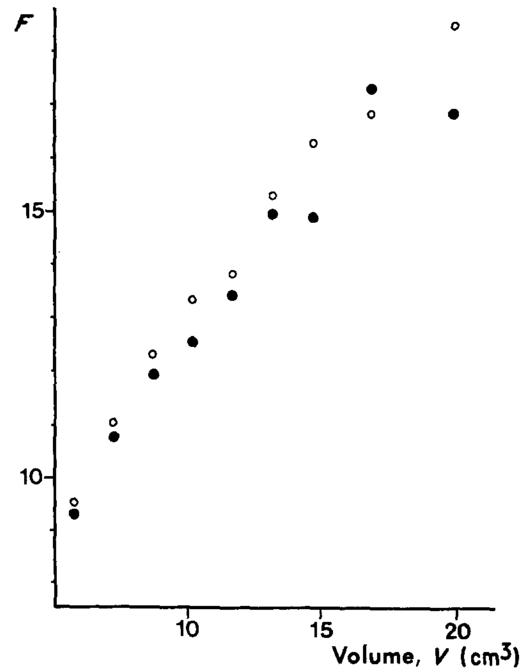

Figure 6 Average number of faces in grains with a given volume. The results of two compressions are shown separately. (●) First compression, (○) second compression.

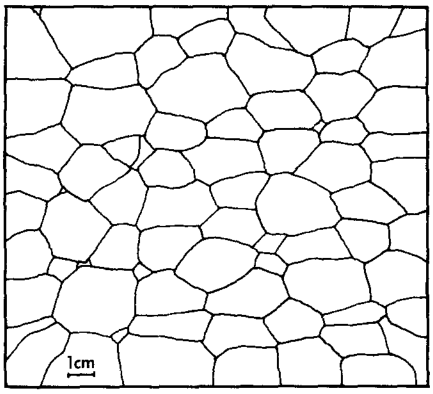

Figure 7 Grains in a section of type 1 (see Fig. 2) in the plasticine lump.

the corresponding curves for the 3-D structure, shown in Figs. 1 and 4, respectively.

Table I shows additional data obtained for the three sections, which includes:

(i) the second moment μ_2 of the frequency distribution $f(i)$; μ_2 is the average value of $(i - 6)^2$ and is a measure of the dispersion around the average value $\bar{i} = 6$.

(ii) the average area per grain $\bar{A}$ and the average grain diameter $\bar{D} = (4\bar{A}/\pi)^{1/2}$.

(iii) the average line intersect $\bar{l}$ ($\bar{l} = 1/P_L$).

The average area is determined from P_A, the number of 2-D vertices per unit area, with $P_A = 2/\bar{A}$. The variation of $\bar{A}$ and $\bar{l}$ from section to section (Table I) is as expected. Using standard equations of stereology, the total length L_V of 3-D edges and the total area S_V of grain boundaries, both per unit volume, can be determined from the average values of P_L and P_A. We found $L_V = 1.21\,\text{cm}^{-2}$ and $S_V = 1.26\,\text{cm}^{-1}$. These values have been used to test the following equation recently derived by Hanson [10] to obtain the average grain volume from 2-D observations

TABLE I Parameters of planar sections

Section type	μ_2	$\bar{A}$ (cm^2)	$\bar{D}$ (cm)	$\bar{l}$ (cm)	a
1	2.047	2.96	1.94	1.47	0.931–0.926
2	2.572	3.33	2.06	1.56	1.107–1.115
3	2.700	3.78	2.19	1.76	1.069–1.065
Mean value	–	3.36	2.06	1.59	–

$$\bar{V} = \left(\frac{4.83}{L_V^{1/2}} - \frac{2.9104}{S_V}\right)^3 \qquad (2)$$

The equation gives $\bar{V} = 9.1\,\text{cm}^3$ which compares very well with the measured volume $\bar{V} = 8.8\,\text{cm}^3$.

Finally determinations of $m(i)$ were also made; $m(i)$ is the average number of sides in polygons adjacent to polygons with i sides. The intention was to test the following relation according to Aboav [12] and Weaire [13]

$$m(i) = 6 - a + \frac{6a + \mu_2}{i} \qquad (3)$$

where a is a constant. The linear relation on $1/i$ is fairly well obeyed for any of the sections, as shown in Fig. 11. The values of a are indicated in Table I; in each case, the first value was determined from the slope and the second from the intercept of the straight lines of Fig. 11.

5. Conclusion

The potentialities of a plasticine model of a polycrystal in studies of topological properties have been illustrated in experiments in which a log-normal distribution of grain volumes was used. The main advantages of this model, compared to previously used similar models, are the possibility of choosing the grain size distribution and of making studies in planar sections of the polycrystal which can then be correlated

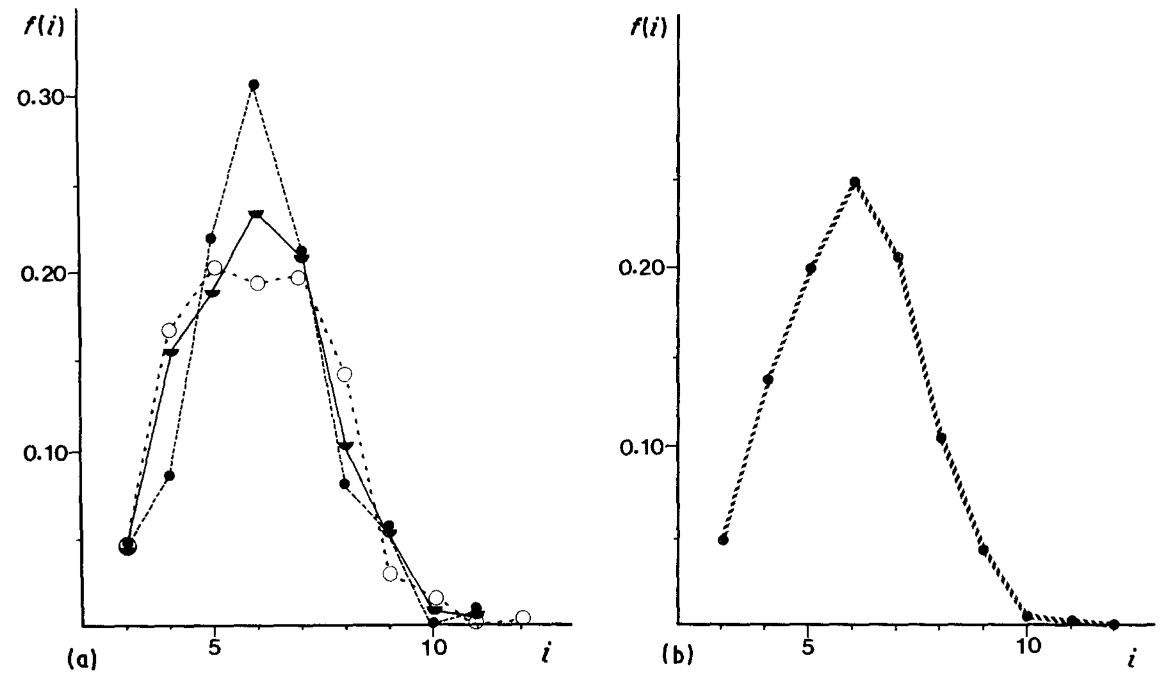

Figure 8 (a) Frequency f of polygonal grains with i sides in planar sections of each of the types indicated in Fig. 2. Section type ●, 1; ▾, 2; ○, 3. (b) Average frequency of i-sided grains; the average is the arithmetic mean for the three types of sections.

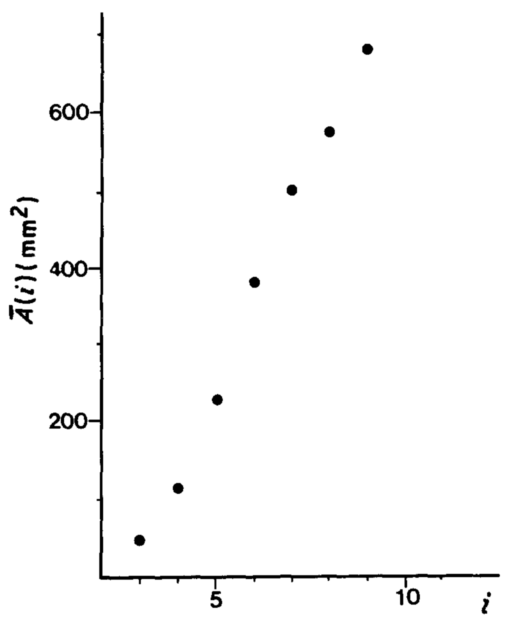

Figure 9 Average area of grains with i sides in the three sections.

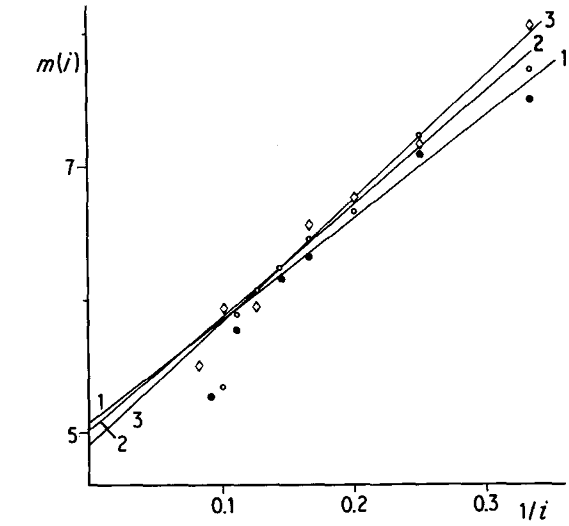

Figure 11 The average number of sides, $m(i)$, in grains adjacent to i-sided grains, in planar sections of each type, plotted as a function of $1/i$. The straight lines were determined by a standard best fitting method. Section type: ●, type 1; ○, type 2; ◇, type 3.

with the 3-D determinations. Another not insignificant advantage is the possibility of determining the average volume per grain, a quantity that cannot be obtained with precision from 2-D observations.

The model has some disadvantages. The first is that it probably cannot reproduce all grain and biological cell structures. In particular the faces are curved, a characteristic that has not been mentioned in the literature describing similar models. The structure obtained is analogous to the Johnson–Mehl structure [9, 14], including the average $\bar{F}$. The diameter of a ball is probably related to the "time of nucleation" parameter used in the Johnson–Mehl model, although in this model the nucleation sites are randomly distributed in space and the grain volume distribution is not log-normal.

The fact that the plasticine polycrystal is oriented, due to the uniaxial deformation, implies that differently oriented sections will lead to different parameters, requiring some averaging in order to correlate with the 3-D parameters. This can be regarded as an advantage if one wishes to study the anisotropy of 2-D sections in oriented structures.

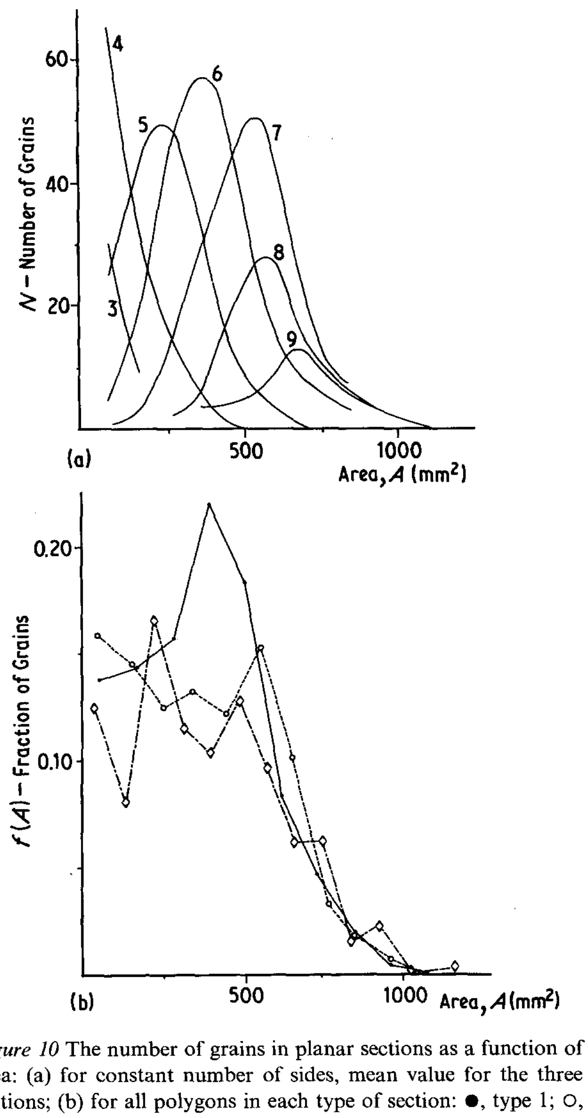

Figure 10 The number of grains in planar sections as a function of area: (a) for constant number of sides, mean value for the three sections; (b) for all polygons in each type of section: ●, type 1; ○, type 2; ◇, type 3.

References

1. J. W. MARVIN, *Amer. J. Bot.* **26** (1939) 280.
2. E. B. MATZKE, *ibid.* **26** (1939) 288.
3. J. E. BERNAL, *Nature* **17** (1959) 141.
4. *Idem, Proc. R. Soc.* **280A** (1964) 299.
5. E. B. MATZKE, *Amer. J. Bot.* **33** (1946) 58.
6. F. N. RHINES, K. R. CRAIG and D. A. ROUSSE, *Met. Trans.* **7A** (1976) 1729.
7. W. N. WILLIAMS and C. S. SMITH, *Trans. AIME* **194** (1952) 755.
8. C. S. SMITH, "Metal Interfaces" (American Society of Metals, Cleveland, Ohio, 1952) p. 65.
9. K. W. MAHIN, K. HANSON and J. W. MORRIS Jr, *Acta Metall.* **28** (1980) 443.
10. K. L. HANSON, *ibid.* **27** (1979) 515.
11. E. E. UNDERWOOD, in "Quantitative Microscopy", Ch. 4, edited by R. T. DeHoff and F. N. Rhines (McGraw-Hill, New York, 1968) p. 77.
12. D. A. ABOAV, *Metallography* **3** (1970) 383.
13. D. WEAIRE, *ibid.* **7** (1974) 157.
14. W. A. JOHNSON and R. F. MEHL, *Trans. AIME* **135** (1939) 416.

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