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STEREOLOGICAL PARAMETERS OF MODEL POLYCRYSTALLINE STRUCTURES BUILT FROM POLYHEDRA OF VARIOUS SHAPE AND SIZE

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ABSTRACT

The five selected models of polycrystalline microstructure proposed by Williams (1979), built from polyhedra of various shape and size as well as a model of homogenous microstructure (a set of truncated octahedra of the same size) have been compared in this work. All the elements of the models containing approximately 18000 polyhedra have been entirely determined in 3-D space. On the basis of 8000 random plane section of the model microstructures (7000000 plane sections of polyhedra) the "statistical" and "geometrical" distributions of parameters characterizing grain size and shape in 2-D space were evaluated. The studies indicated that "statistical" and "geometrical" distributions that describe both size and shape of grains in 3-D and 2-D space contain significantly different information concerning the model polycrystalline structures. It was shown that "geometrical" distribution of grain plane section area is more suitable for grain size evaluation of inhomogeneous granular structures than "statistical" one. It was stated-out that neither the distribution of number of sides of polygons obtained on plane sections of the model structures nor the distribution of polygons form factor are clearly related to the shape of polyhedra forming the model structures.

Key words: grain size, computer simulation and modelling.

INTRODUCTION

The goal of the research programme presented in the paper (Cwajna, 1993) is to work out a data base for 3-D granular microstructure analysis derived from 2-D data obtained for the investigated material with an automatic image analyser. One of the elements of this data base are 3-D and 2-D characteristics of model polycrystalline structures containing polyhedra of various shape and size, proposed by Williams (1979). The models are the subject of the investigation in this work.
It has been assumed that the results obtained for Williams' models will make it possible to evaluate also the accuracy of measures of average grain size as well as of grain size inhomogeneity, presented in our previous works (Cwajna et al 1987, Maliński et al 1988, 1991 a, b).

TOPOLOGICAL AND GEOMETRICAL CHARACTERISTIC OF WILLIAMS' MODEL POLY-CRYSTALLINE STRUCTURES

Taking into account the results of the survey of literature data on grain size and shape of polycrystalline materials done in the work (Maliński et. al, 1988) as well as Aboav's (1991) suggestions relating to probable grains shape in granular microstructures, the following Williams'

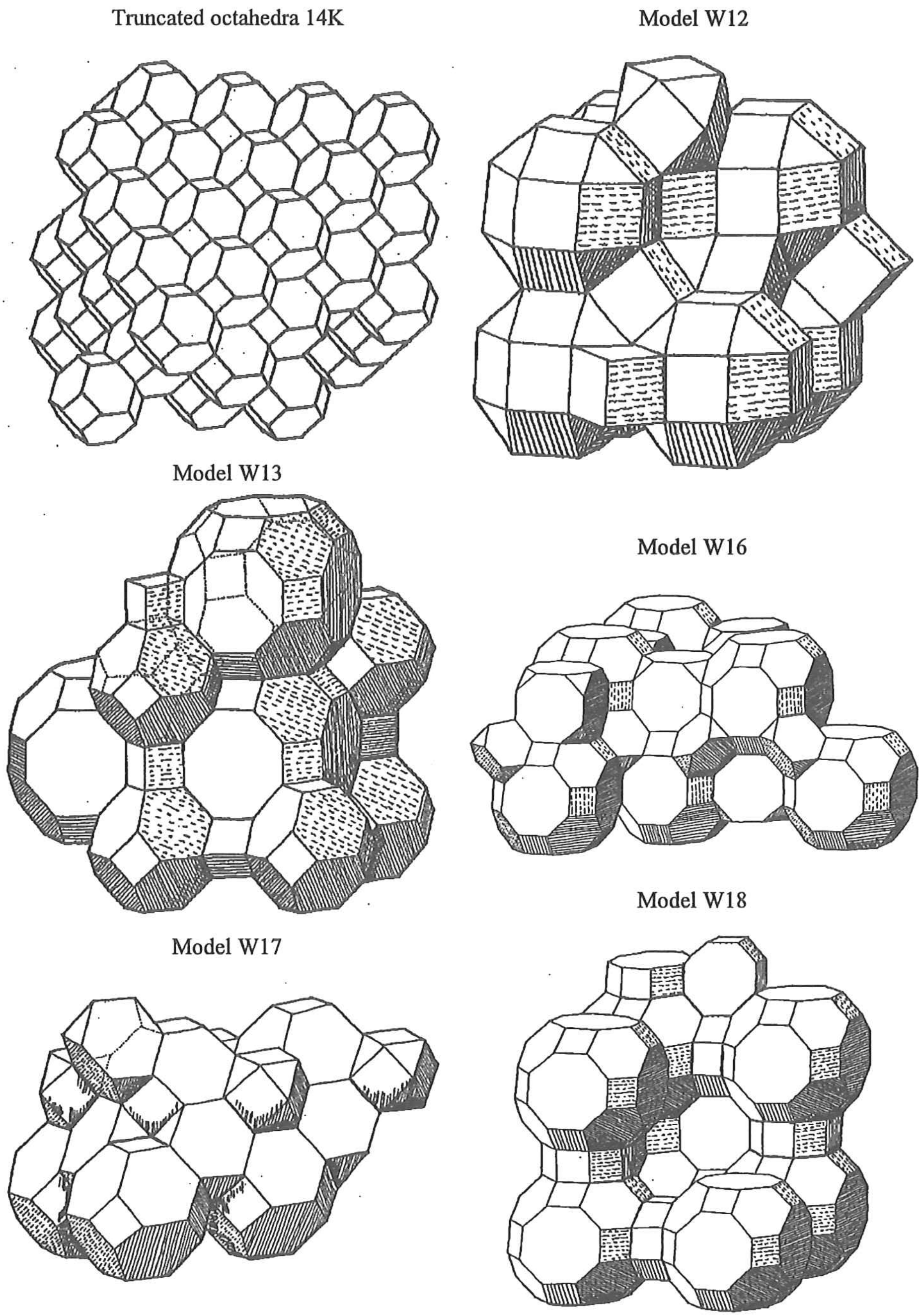


Fig. 1. Set of truncated octahedra of the same size and Williams' model polycrystalline structures.

models have been selected for the study (Fig. 1):

- 6 connected network of cubes, cuboctahedra and small rhombicuboctahedra with packing ratio 3:1:1 (model W12),
- 4 connected network of cubes, truncated octahedra and great rhombicuboctahedra with packing ratio 3:1:1 (model W13),
- 4 connected network of truncated tetrahedra, truncated cubes and great rhombicuboctahedra with packing ratio 2:1:1 (model W16),
- 5 connected network of truncated tetrahedra, truncated octahedra and cuboctahedra with packing ratio 2:1:1 (model W17),
- 4 connected network of octagonal prism and great rhombicuboctahedra with packing ratio 3:1 (model W18).

Topological parameters of the models are collected in Table 1. Models W16 and W18 have the same topological characteristic as truncated octahedron has although they are composed of polyhedra of various shape (Fig. 2).

Table 1. Topological characteristic of the model polycrystalline structures

Topological parameter	Model structures					
	TO	W12	W13	W16	W17	W18
Number of faces	14.00	11.60	11.60	14.00	11.00	14.00
Number of edges	36.00	21.60	28.80	36.00	24.00	36.00
Number of corners	24.00	12.00	19.20	24.00	15.00	24.00
Average value of edges per face	5.143	3.724	4.966	5.143	4.364	5.143
Number of edges meeting at a corner	3.0	m.v. 3.6	3.0	3.0	m.v. 3.2	3.0
Dihedral angle	m.v. 120.0	m.v. 120.0	m.v. 120.0	m.v. 120.0	m.v. 112.5	m.v. 120.0
Corner angle	m.v. 110.0	m.v. 83.(3)	m.v. 107.5	m.v. 110.0	m.v. 97.5	m.v. 110.0

Notes: m.v. - mean value.

The data obtained for all the models, particularly for the models W12 and W13, show that "statistical" and "geometrical" distributions give quite different quantitative description of grain shape in the inhomogeneous granular structures. The most common polyhedra are those with small number of faces, but the largest volume fraction occupy the polyhedra with great number of faces.
The models have visibly different distributions of polyhedra volume (Fig. 3). It is worth to be noticed that they are the rather specific models of inhomogeneous granular structures with only 2 or 3 grain size classes.

COMPARISON OF 3-D AND 2-D PARAMETERS DESCRIBING GRAIN SIZE AND SHAPE OF MODEL STRUCTURES

With an application of computer simulation technique presented in detail in (Maliński, 1985), and based on Miles and Davy (1976) concept of random sectioning of polyhedra, for the model structures built from approximately 18000 polyhedra, the "statistical" and "geometrical" distributions of grain size and shape in 2-D space were determined. The number of random sections of the models was 8000, what made the number of grain plane section ~7000000. The distributions that describe grain size of models in 2-D space are shown in Fig. 4. Kolmogorov-Smirnov's test of goodness of fit testifies that all the distributions are significantly different.

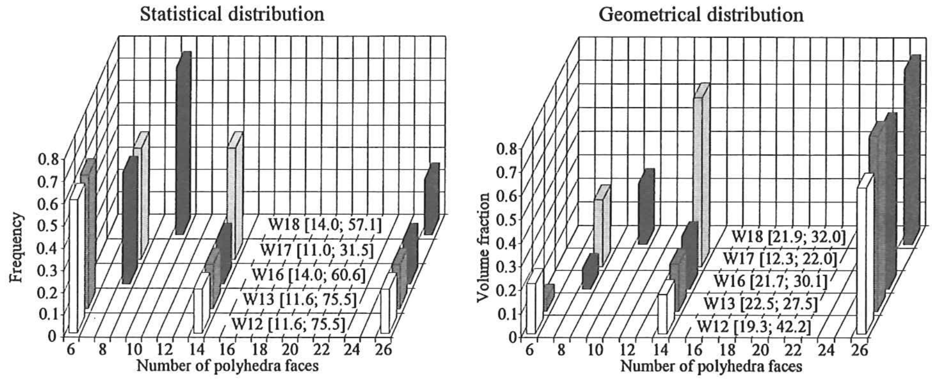


Fig. 2. Distributions of number of polyhedra faces in the Williams' model polycrystalline structures [mean value; equivalent coefficient of variation [%]].

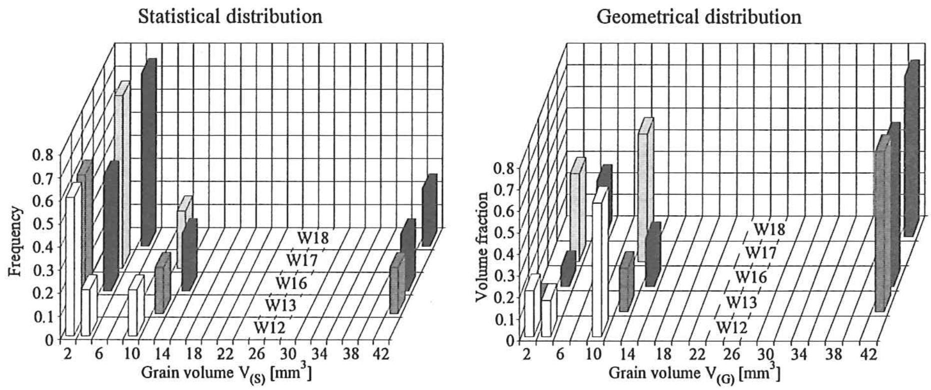


Fig. 3. Distribution of true grain volume ("statistical") and volume-weighted grain volume ("geometrical") of model structures (data for polyhedra edge length = 1mm).

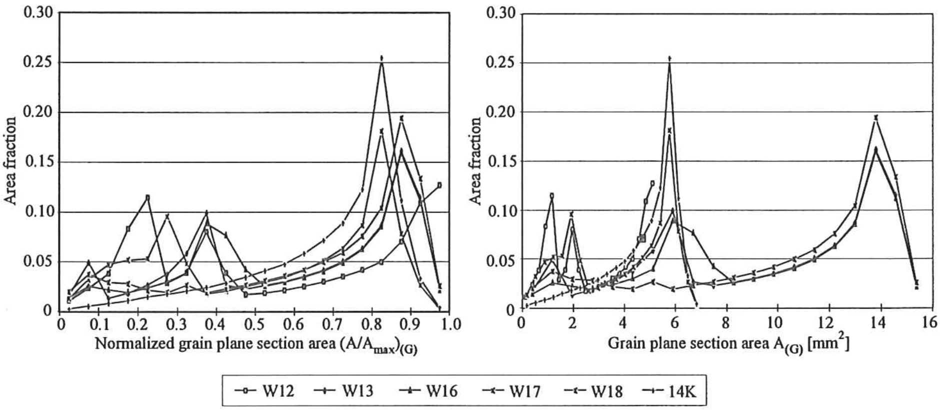


Fig. 4. "Geometrical" grain size distribution of model structures in 2-D space.

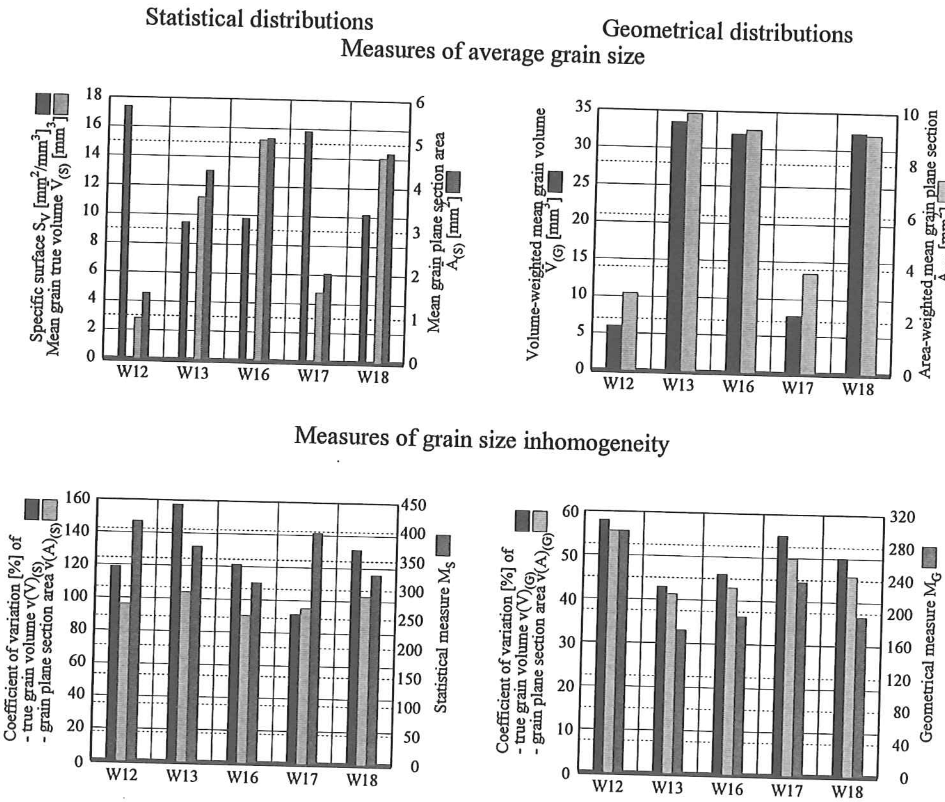
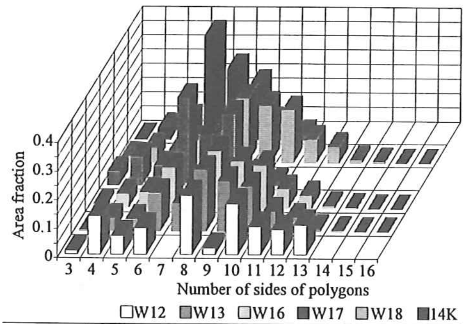


Fig. 5. Comparison of "statistical" and "geometrical" measures of average grain size and size inhomogeneity in 3-D and 2-D space of Williams' model polycrystalline structures (data for polyhedra edge length = 1mm). $M_{S,G}$ - measures of grain size inhomogeneity obtained by testing the goodness of fit of the given Williams' model and the distribution determined for homogenous granular structure built of truncated octahedra of the same size (Maliński et al., 1991a).

The comparison of measures of average grain size as well as of grain size inhomogeneity of investigated models in 3-D and 2-D space, presented in Fig. 5, indicates that:

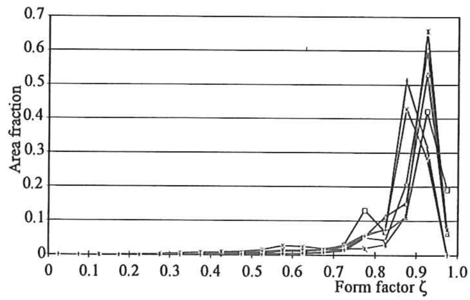
1. The conclusions that can be drawn from the analysis of parameters of 2-D grain size geometrical distribution [$\overline{A}_{(G)}$, $v(A)_{(G)}$, M_G] are entirely consistent with those taken from direct comparison of parameters of grain volume distribution function [$\overline{V}_{(G)}$, $v(V)_{(G)}$]. Stereological parameter M_G is a more sensitive measure of grain size inhomogeneity than the coefficient of variation $v(A)_{(G)}$.
2. There exists an unequivocal relationship between the statistical measures of average grain size in 2-D and 3-D space $\overline{A}_{(S)}$ and $\overline{V}_{(S)}$, whereas the measures of grain size inhomogeneity $v(A)_{(S)}$ and M_S do not correspond with the grain volume coefficient of variation $v(V)_{(S)}$. This finding does not agree well with the result of our previous study of computer simulated structures with larger number of grain size classes and smaller grain size variation (Maliński et. al, 1991 a, b).
3. The data obtained for the models of similar average grain size: W13, W16 and W18 confirm that the specific surface of grain boundaries S_V is a grain size and shape dependent parameter.

Therefore it seems reasonable to suggest the application of the area-weighted mean plane section area $\overline{A}_{(G)}$ as a measure of average grain size and parameter M_G or coefficient of variation $v(A)_{(G)}$ as a measure of grain size inhomogeneity of inhomogeneous granular structures.



	W12	W13	W16	W17	W18	14K
mean value $\bar{A}$	8.57	8.28	8.11	6.45	8.48	6.72
equivalent coefficient of variation [%]	34.4	25.1	27.1	24.4	25.8	18.7

Fig. 6. Area fraction of polygons of various shape on the plane section of model structures.



	W12	W13	W16	W17	W18	14K
mean value $\bar{\zeta}$	0.882	0.903	0.879	0.836	0.885	0.878
equivalent coefficient of variation [%]	10.5	7.1	11.3	15.6	14.1	6.63

Fig. 7. Area fraction of polygons of various shape factor $\zeta=\pi A/4P^2$ (A-area, P-perimeter) on plane section of model structures.

A detailed analysis of the distributions commonly used as a grain shape characteristic in 3-D (Fig. 2) and 2-D space (Fig. 6 and 7) shows that there is not distinct relationship between the shape of polyhedra forming the granular structure and the distribution of number of sides of polygons obtained on plane section of this structure as well as the distribution of polygons form factor ζ. Hence, the problem of quantitative evaluation of grains shape is still insoluble.

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REFERENCES

Aboav AD. The stereology of the intergranular surface of metal. In: Proc. 3rd Conference "Stereology in Materials Science and Engineering", Szczyrk, Poland, 1990: 119-130.

Cwajna J. Quantitative structural criteria of steel quality control. In: Proc. 6th European Congress for Stereology, Prague, 1993.

Cwajna J, Maciejny A, Maliński M. Stereological criteria and measures of structural stability of one-phase polycrystalline materials. Acta Stereol 1987; 6/III: 261-6.

Maliński M. Stereological criteria of grain size homogeneity of one-phase materials. Doctor's Thesis. Silesian University of Technology, Faculty of Metallurgy. Katowice, Poland, 1985.

Maliński M, Cwajna J, Maciejny A. Stereological criteria and measures of grain size homogeneity. In: The stereological methods in materials science. Prace Komisji Metalurgiczno-Odlewniczej PAN, Metalurgia 35, 1988: 43-56.

Maliński M, Cwajna J, Chrapoński J. Grain size distribution. Acta Stereol 1991a; 10/1: 73-82.

Maliński M, Cwajna J, Chrapoński J. 3-D and 2-D stereological parameters of computer simulated grain structures. In: Proc. International Conference on Grain Growth in Polycrystalline Materials, Rome, Italy, 1991 b.

Miles RE, Davy P. J Microsc, 1976; 107: 211-6.

Williams R. The geometrical foundation of natural structure. Dover Publications Inc., New York, 1979.