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GRAIN SIZE DESCRIPTION - RELATIONSHIPS BETWEEN 2D AND 3D PARAMETERS

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ABSTRACT

2D and 3D morphological and stereological parameters of computer simulated models of microstructure of one phase polycrystalline materials are presented.

The study of the models of homogenous microstructures built from polyhedra of the same size and shape (sets of truncated octahedra, Williams' β–tetrakaidecahedra and rhombic dodecahedra) has shown that the model of plane section of equilibrium materials in the form of set of regular hexagons, presented in basic literature on physical metallurgy and materials science is irrelevant. 2D parameters and representative plane sections of models of homogenous microstructure were shown.

The models of inhomogenous polycrystalline microstructures built from polyhedra of various size and shape – Williams' models, cell models and Johnson–Mehl models, were used for determination of empirical equation between mean plane section area of grains $E_N(A)$ and mean grain volume $E_N(V)$ as well as between coefficient of variation of grains plane section area $CV_N(A)$ and coefficient of variation of grain volume $CV_N(V)$.

These equations may be the basis of the simple method for the determination of parameters of grain volume distribution.

Key words: 3D modelling, stereology, grain size.

INTRODUCTION

Computer simulated 3D models of materials microstructure precisely described in 2D and 3D spaces are widely applied for:

- verification of correctness of polycrystalline materials models applied in theory of materials properties,
- assessment of precision and versatility of hitherto used methods for the determination of grains or particles volume distribution as well as for estimation of other stereological parameters,
- searching for new relations between parameters of plain and spatial materials microstructure and elaboration of new stereological methods.

There are numerous works dealing with various applications of the computer simulated models of polycrystalline materials. They were quoted in our review works (Maliński 1985, Cwajna et al. 1993, Cwajna 1994, Chrapoński 1997). This paper and the other two related paper published in the same proceedings (Chrapoński et al. 1998, Maliński et al. 1998) presents our own experiences in this field.

REPRESENTATIVE PLANE SECTIONS OF MODELS OF HOMOGENOUS GRANULAR MICROSTRUCTURE

The results of the evaluation of the degree to which the most commonly accepted polyhedra satisfy the topological and thermodynamic criteria of structural stability were presented in our previous works (Maliński 1985, Cwajna et al. 1986, Cwajna et al. 1993). They indicate that the most functional model is built of truncated octahedra of the same size (Fig. 1).

These representative plane section of this 3D model (Fig. 1b) is built from the polygons of various size and shape and it is its very characteristic feature. The degree of polygons size inhomogeneity is strictly definite. The model of plane section of equilibrium materials microstructure in the form of set of regular hexagons, presented in basic literature on physical metallurgy and materials science, is therefore irrelevant. This also concerns the newest model proposed by Ashby and Jones (1986) – Fig. 2.

The distribution of parameters usually used for grain size description in 2D space determined for the model homogenous microstructure made it also possible to propose new stereological criteria and measures of grain size inhomogeneity (Cwajna et al. 1987, Maliński et al. 1992).

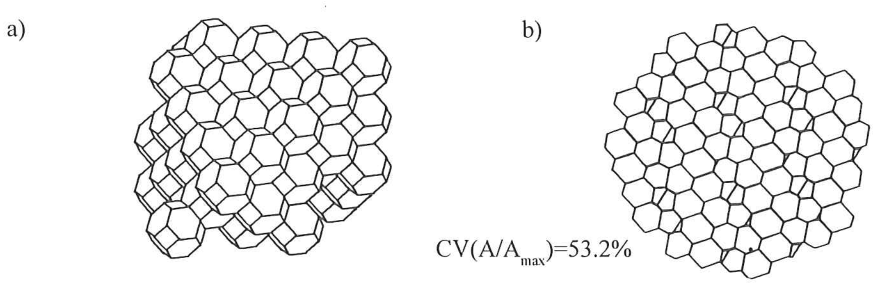

Fig. 1. Model of homogenous granular microstructure: a) agregate of grains, b) representative plane section. $CV(A/A_{max})$ – coefficient of variation of relative plane section area.

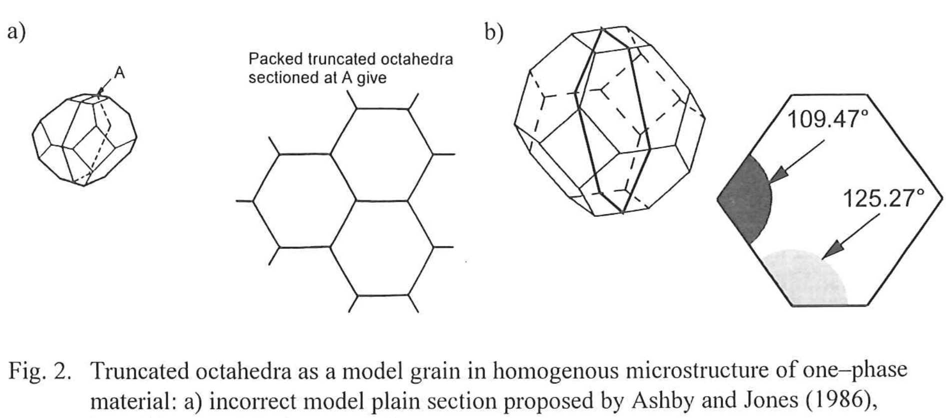

Fig. 2. Truncated octahedra as a model grain in homogenous microstructure of one–phase material: a) incorrect model plain section proposed by Ashby and Jones (1986), b) Ashby's model after correction.

APPLICATION OF 3D MODEL OF POLYCRYSTALLINE STRUCTURES FOR THE DETERMINATION OF RELATIONSHIPS BETWEEN 3D AND 2D PARAMETERS DESCRIBING GRAIN SIZE

Grain size of polycrystalls is the oldest structural criterion applied in materials quality control. There exist commonly accepted opinion, that the volume distribution or its parameters are the most natural description of grain size of polycrystalline materials (Kurzydłowski and Ralph, 1995).

Simultaneously the data showing that the versatile and accurate stereological methods for quantitative evaluation of granular materials microstructure at acceptable labour consumption and cost has not been work out yet (Czarski et al. 1996, Chrapoński et al. 1997, Chrapoński et al. 1998).

In the study which goal was the determination of empirical relationships between 3D and 2D parameters of granular microstructure three groups of computer simulated models were applied:

- the sets of regular polyhedra of various size and shape proposed by Williams (1979) – Fig. 3,
- cell models – Fig. 4,
- Johnson–Mehl models – Fig. 5.

The methods of creation of these models are presented in (Chrapoński 1997, Maliński and Chrapoński 1997, Chrapoński and Maliński 1997, Maliński et al. 1998).

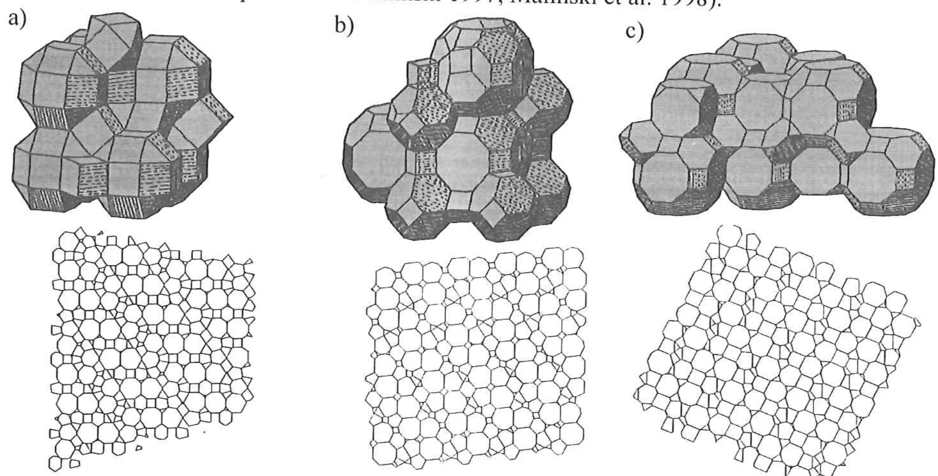

Fig. 3. Model Williams' structures and their random plane sections: a) W1 structure, b) W2 structure, c) W3 structure.

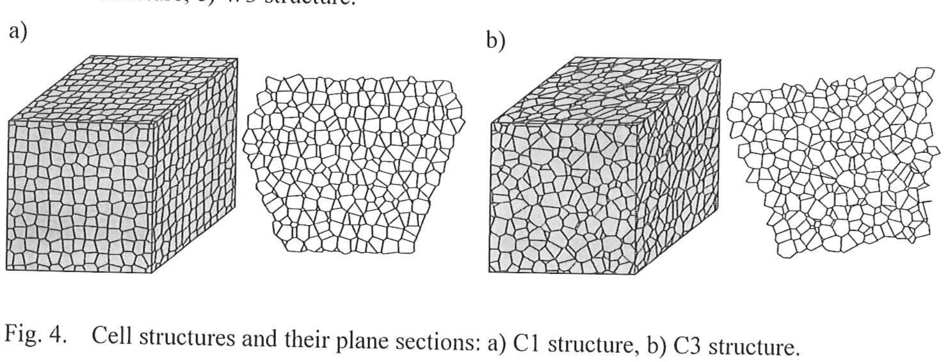

Fig. 4. Cell structures and their plane sections: a) C1 structure, b) C3 structure.

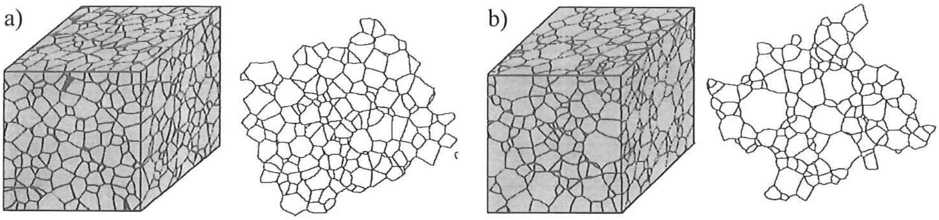

Fig. 5. Selected Johnson-Mehl's models of polycrystalline materials microstructure and their random plane sections: a) model structure JM1, b) model structure JM3.

The comparison of the random plane section of the computer simulated models and of metallic materials, engineering ceramic and composites (Fig. 6) as well as the analysis of 2D parameters of the models and of the real materials (Table 1) indicate, that the models satisfactory present the microstructure of engineering materials.

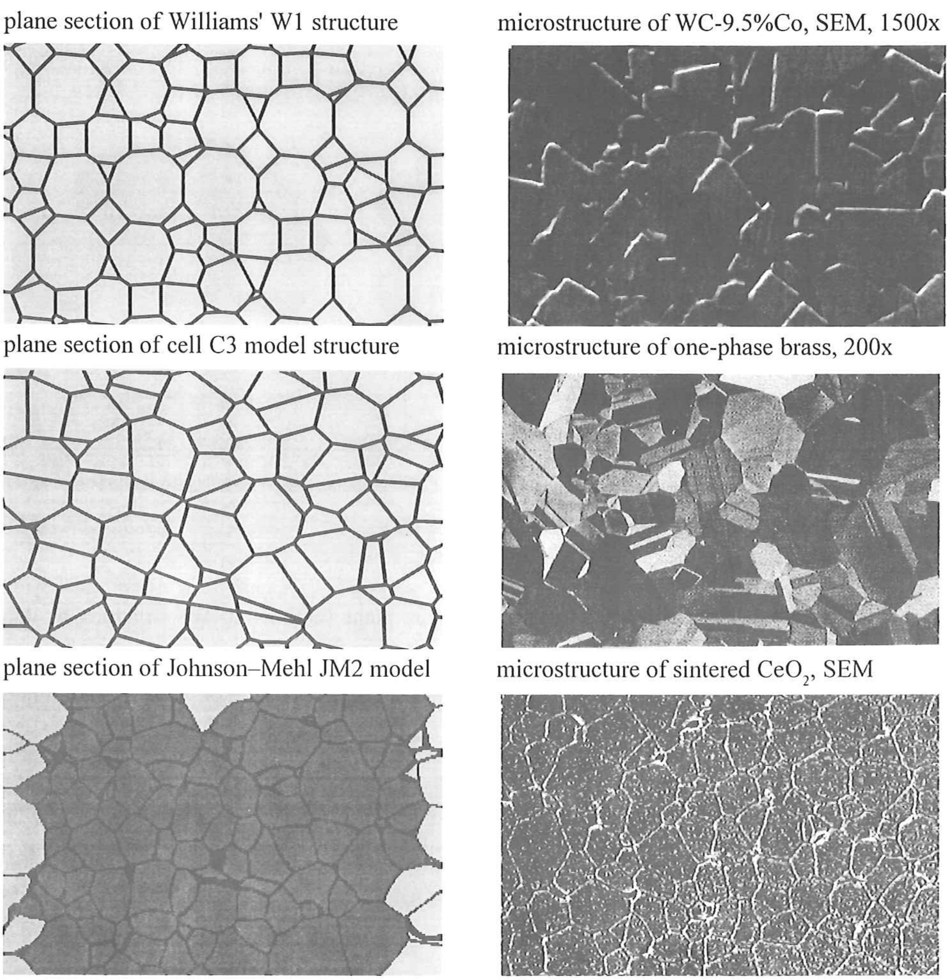

Fig. 6. Comparison of random plane sections of model structures and microstructures of real materials.

Table 1. Comparison of standard deviation of parameters describing grain size in 2D and 3D spaces of model structures as well as of real materials microstructure

Material	SD(lnV)	SD(lnA)
Al	1.06÷1.45	1.1÷1.35
316L steel	1.03÷1.47	1.3÷1.4
Ti-α	0.95	0.95
Fe-α	1.16	0.95
Fe-α (selective grain growth)	1.82	1.39
Johnson-Mehl model structures		
JM1	0.75	1.33
JM2	0.96	1.27
JM3	1.01	1.51

On the basis of the data obtained in computer simulation study of models described in (Chrapoński 1997, Maliński et al. 1998) relationships between 2D and 3D measures of mean grain size as well as of size inhomogeneity were determined – Fig. 7 and 8. The equation:

$$E_N(V)=1.628\ E_N(A)^{1.508} \quad (1)$$

is similar to this, presented by Nunez and Domingo (1988):

$$E_N(V)=C\ E_N(A)^{3/2} \quad (2)$$

as well as to this for the models obtained by spatial Poisson–Voronoi tessellation (Hahn and Lortz, 1994):

$$E_N(V)\cong 1.76\ E_N(A)^{3/2} \quad (3)$$

The calculated value of constant C for the investigated models (Chrapoński 1997, Cwajna et al. 1997) has show that C is the grain shape and size inhomogeneity dependent factor.

The equations presented in Fig. 7 and 8 may be the basis of the simple method for the determination of parameters of grain volume distribution. However these relationships should be verified in the study of larger number of models of strongly diversed grain volume distributions as well as for the models with bimodal grain size distribution.

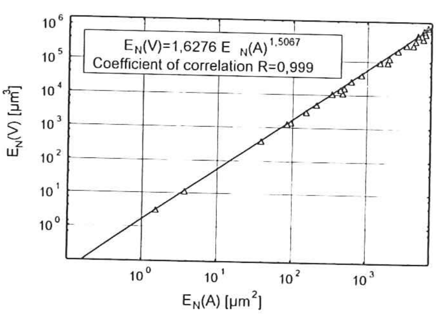

Fig. 7. Relationship between mean plane section area of grains $E_N(A)$ and mean grain volume $E_N(V)$.

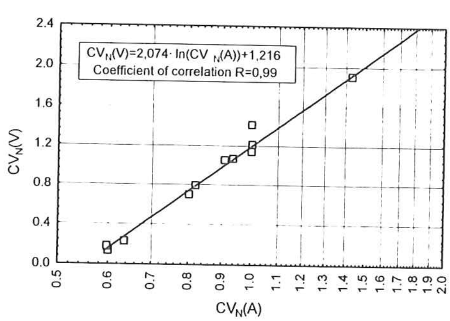

Fig. 8. Relationship between coefficient of variation of grains plane section area $CV_N(A)$ and coefficient of variation of grain volume $CV_N(V)$.

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REFERENCES

Ashby MF, Jones DRH. Engineering Materials 2 – An Introduction to Microstructures, Processing and Design. Oxford, New York, Beijing, Frankfurt, Sao Paulo, Sydney, Tokyo, Toronto: Pergamon Press 1986.

Chrapoński J. Usefulness evaluation of the stereological methods applied for grain size assesment in polycrystalline materials. PhD thesis. Silesian University of Technology, Faculty of Materials Engineering, Metallurgy and Transportation, Katowice, Poland, 1997 (in polish).

Chrapoński J, Cwajna J, Maliński M. Estimation of grain size. Part III: point sampled intercepts and disector. In: Proc. of International Conference on The Quantitative Description of Materials Microstructure QMAT-97. Warsaw 1997: 229–34.

Chrapoński J, Maliński M. 3D modelling of polycrystalline grain structures. Part II: Johnson–Mehl structures. In: Proc. of International Conference on The Quantitative Description of Materials Microstructure QMAT-97. Warsaw 1997: 391–96.

Chrapoński J, Maliński M, Cwajna J. Usefulness evaluation of the stereological methods applied for grain size estimation. 7 ECS. Amsterdam: 1998.

Cwajna J. Quantitative structural criteria of steel quality control. Acta Stereol 1994; 13/2: 409–25.

Cwajna J, Maciejny A, Maliński M. Stereological criteria of grain size homogeneity. In: Proc. 7th Riso International Symposium on Metallurgy and Materials Science "Annealing Processes – Recovery, Recrystallization and Grain Growth", 1986: 273-8.

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.

Cwajna J, Maliński M, Szala J. Grain size as a structural criterion of polycrystalline materials quality. Inżynieria Materiałowa 1993; 4: 79–80 (in polish).

Czarski A, Satora K, Ryś J. Quantitative description of Armco steel structure. Inżynieria Materiałowa 1996; 6: 191-4 (in polish).

Hahn U, Lortz U. Stereological analysis of the spatial Poisson–Voronoi tessellation. J Microsc 1994; 175: 176–85.

Kurzydłowski JK, Ralph B. The quantitative description of the microstructure of materials. Boca Raton, New York, London, Tokyo: CRC Press, 1995.

Maliński M. Stereological criteria of grain size homogeneity of one–phase materials. PhD thesis. Silesian University of Technology, Faculty of Metallurgy, Katowice, Poland, 1985 (in polish).

Maliński M, Chrapoński J. 3D modelling of polycrystalline grain structures. Part I: Williams' and cell structures. In: Proc. of International Conference on The Quantitative Description of Materials Microstructure QMAT-97. Warsaw 1997, 383–90.

Maliński M, Chrapoński J, Cwajna J. Algorithms for 3D modelling of polycrystalline structures. 7 ECS. Amsterdam: 1998.

Maliński M, Cwajna J, Chrapoński J. 3D and 2D stereological parameters of computer simulated grain structures. Materials Science Forum 1992; 94-96: 285–94.

Williams R. The geometrical foundation of natural science. New York: Dover Publications 1979.

Presented at the 7th European Congress for Stereology, Amsterdam, April 20th to 23rd, 1998.