Modelling of Polycrystalline Microstructures Represented by Space-filling Polyhedral Cellular Systems

Tamás Réti

Budapest Polytechnic, Doberdó u. 6, H-1031 Budapest, Hungary

E-mail: reti.tamas@bgk.bmf.hu

Imre Felde

Bay Zoltán Institute for Materials Science and Technologies, Fehérvári u. 130., H-1116 Budapest, Hungary

E-mail: felde@bzaka.hu

Gustavo Sanchez Sarmiento

Universidad de Buenos Aires, Facultad de Ingenieria, Av. Paseo Colon 850, (1063) Buenos Aires, Argentina

E-mail: Sanchezsarmiento@arnet.com.ar

Rafael Colás

Facultad de Ingeniería Mecánica y Eléctrica, Universidad Autónoma de Nuevo León, Pedro de Alba s/n Cd. Universitaria, 66450 San Nicolás de los Garza, N.L. MEXICO

E-mail: rcolas@ccr.dsi.uanl.mx

Abstract: In order to characterize topologically the polycrystalline microstructure of single-phase alloys computer simulations are performed on 3-dimensional cellular models. These infinite periodic cellular systems are constructed from a finite set of space filling convex polyhedra (grains). It is shown that the appropriately selected topological shape factors can be successfully used for the quantitative characterization of computer-simulated microstructures of various types.

1. Introduction

Three-dimensional random or periodic cellular systems are generally used to model the geometric structure of many natural and engineered materials [1,2,3,4]. This is due to the fact, that topologically, the 3-D polycrystalline microstructure of a single-phase alloy is considered as a partition of the space into regular or irregular polyhedra [5,6]. Consequently, a 3-D polycrystalline microstructure can be simply modelled by a cellular system composed of polyhedral-shaped cells.

This paper presents a method which enables the topological classification of 3-D cellular systems designated to the microstructural modelling of single-phase polycrystalline alloys. The novel approach is based on the introduction of the so-called topological shape factors computed from the scalar topological invariants of the cellular systems.

The applicability of the method has been tested using a finite set of 3-D periodic space-filling polyhedral systems. Investigations based on computer simulation suggest that the proposed method is an efficient tool for the topological evaluation of polycrystalline structures modelled by infinite periodic polyhedral systems.

2. Global topological characteristics of 3-D periodic cellular systems

Infinite periodic cellular structures are simple and ideal systems to analyse the topological properties of polycrystalline materials. As it is known each 3-D infinite periodic cellular system composed of convex polyhedra can be represented by a torus, and as a result of this topology preserving mapping a so-called finite toroidal cellular system can be generated [7,8,9]. It can be verified that for a 3-D finite toroidal cellular system (FTC system) constructed from a finite set of unit domains the Euler-equation is valid in the following form:

$$-N+F-E+V=0 \tag{1}$$

In Eq.(1), N is the number of cells (polyhedra), F is the number of faces, E is the number of edges, and V is the number of vertices, respectively. The total number N of cells is $N=\sum N_f$ where N_f is the number of f-sided cells (f=4,5,... f_{max}). The fraction (or frequency) p_f of f-faceted cells is $p_f = N_f/N$, where $p_f>0$. Consequently, $\sum p_f$ =1. For FTC systems, the average number of faces per cell denoted by $\langle f\rangle$ is defined as $\langle f\rangle = \sum fp_f$, and the second moment of face number per cell can be calculated as $\langle f^2\rangle = \sum f^2 p_f$. Consequently, the variance $\mu(f)$ of number of faces per cell is given as $\mu(f) = \langle f^2\rangle - \langle f\rangle^2$. A 3-D cellular system is called homogenous (face- homogenous) if $\mu(f)=0$. Since any 2-dimensional face is a common face of two different neighbor cells, one obtains $N\langle f\rangle=2F$.

In FTC systems, for each vertex X, the number of edges incident on X is called the valency of X, and denoted by r (or r(X)). If all of the vertices have the same valency R, then the FTC system is said to be regular or an R-valent system (R=4,5,6,…). Generally, vertices do not all have the same valency, consequently, we may define an average valency [r] as follows:

$$[r]=\frac{1}{V}\sum_{r} rV_r \tag{2}$$

In Eq. (2) V_r is the number of r-valent vertices, for which $V=\Sigma V_r$. From this it follows that for every FC system we have $[r]V=2E$.

The number of faces incident on a common edge can be different. The number of faces incident on edge Y is called the degree of Y, and denoted by d (or d(Y)). For FTC systems, the average degree [ε] of edges is defined as

$$[\varepsilon]=\frac{1}{E}\sum_{d} dE_d \tag{3}$$

In Eq. (3) E_d is the number of edges of degree d, for which $\sum E_d = E$. It can be verified that the average number [n] of edges per face can be calculated as

$$[n]=\frac{1}{F}\sum_{k} kF_k = \frac{\langle fn(f)\rangle}{\langle f\rangle}=\frac{E}{F}[\varepsilon]=[\varepsilon]\frac{[r](\langle f\rangle-2)}{\langle f\rangle([r]-2)} \tag{4}$$

In. Eq.(4) n(f) is the mean number of edges of f-sided polyhedral cells, and F_k is the number of k-sided faces, for which $\sum F_k = F$. From this concept it follows that for FTC systems, the following inequalities are fulfilled: $[r] \geq 4$, $\langle f\rangle \geq 4$, $3 \leq [n] \leq 6-12/\langle f\rangle<6$, $3 \leq [\varepsilon] \leq 6-12/[r]<6$ and $9<[n][\varepsilon]<36$. Moreover, it is easy to see that for 3-D periodic polyhedral systems composed only of trivalent convex polyhedra (where 3 edges are incident on each vertex), we obtain the following result:

$$[n]=6-\frac{12}{\langle f\rangle} \tag{5.a}$$

and

$$[\varepsilon] = 6 - \frac{12}{[r]} \tag{5.b}$$

It is important to note that topological quantities $\langle f \rangle$, [r], [ε] and [n] correspond to the „mean incidence numbers" introduced by Aste and Rivier to characterize D-dimensional random cellular froths constituted of (D-1) dimensional polytopes (D=2,3,4,...) [5,6].

In the following it will be demonstrated that starting with the above formulae it easy to generate so-called topological shape factors which can be applicable to the global structural characterization of 3D periodic cellular systems.

3. Topological shape factors

In order to characterize quantitatively the topological structure of FTC systems, four topological shape factors denoted by Λ, CI, Δ and Ψ have been defined:

$$\Lambda = \frac{F-E}{E} = -1 + \frac{[\varepsilon]}{[n]} = \frac{2([r] - \langle f \rangle)}{[r](\langle f \rangle - 2)} \tag{6}$$

$$CI = \frac{N+F+E+V}{N} = 1 + \frac{\langle f \rangle}{2} + \frac{1}{2}(\langle f \rangle - 2)\left(\frac{[r]-2}{[r]+2}\right) \leq 2\langle f \rangle - 2 \tag{7}$$

$$\Delta = \frac{FE}{4VN} = \frac{\langle f \rangle [r]}{16} > 1 \tag{8}$$

$$\Psi = \frac{N\langle f^2 \rangle}{8F} = \frac{\langle f^2 \rangle}{4\langle f \rangle} = \frac{1}{4}\left(\frac{\mu(f)}{\langle f \rangle} + \langle f \rangle\right) \geq \frac{\langle f \rangle}{4} \geq 1 \tag{9}$$

It can be verified that the following inequalities are valid for the topological shape factor Λ:

$$-\frac{1}{2} < \frac{\langle f \rangle - 4}{4 - 2\langle f \rangle} \leq \Lambda \leq 1 - \frac{4}{[r]} < 1 \qquad (10)$$

From Eqs.(6 and10) it follows that $\Lambda \geq 0$, if $[r] \geq \langle f \rangle$, moreover $\Lambda \leq 0$, if $[r] \leq \langle f \rangle$. Additionally, $\Lambda=0$ if and only if, $\langle f \rangle/[r]=[n]/[\varepsilon]=1$.

4. Analysis of polyhedral cellular systems

In order to evaluate the discrimination performance of the four shape factors, investigations have been performed by using a data base of appropriately selected 3D periodic cellular systems. The majority of them is taken from the book by Williams [10], while the others are artificially constructed periodic systems.

For the tested polyhedral systems, the basic topological quantities ($\langle f \rangle$, [n], [r], [ε]), and the computed values of topological shape factors are summarized in Table 1.

Designation	Number of faces per cell, f	Topological data							
		<f>	[n]	[r]	[ε]	CI	Λ	Ψ	Δ
C-6	6	6	4	6	4	8	0	1.5	2.25
H-8	8	8	4.5	5	3.6	12	-0.2	2	2.5
D-12R	12	12	4	5.3333	3	18	-0.25	3	4
D-12E	12	12	4.667	4.5	3.111	20	-0.333	3	3.375
K-14	14	14	5.143	4	3	26	-0.417	3.5	3.5
MT-4A	4	4	3	14	5.143	4.333	0.714	1	3.5
MT-4B	4	4	3	11.6	4.965	4.417	0.655	1	2.9
MC-6	6	6	4	5.111	3.652	8.571	-0.087	1.5	1.917
M0-8	8	8	3	11	3.273	9.333	0.091	2	5.5
XA-5	5	5	3.6	8	4.5	6	0.25	1.25	2.5
XB-5	5	5	3.2	11	4.364	5.667	0.364	1.25	3.438
XC-5	5	5	3.467	8	4.333	6	0.25	1.25	2.5
X-56	5.6	5.333	3.75	7	4.286	6.667	0.143	1.344	2.333
W12	6, 14, 26	11.6	3.724	6	3	16.4	-0.194	4.224	4.35
W13	6, 14, 26	11.6	4.966	4	3	21.2	-0.396	4.224	2.9
W16	8, 14, 26	14	5.143	4	3	26	-0.417	4.464	3.5
W17	8, 14	11	4.364	5	3.2	17	-0.267	2.955	3.438
W17A	8, 14	11	4.364	5	3.2	17	-0.267	2.955	3.438
W17B	8, 14	11	3.273	8	3	14	-0.083	2.955	5.5
W18	10, 26	14	5.143	4	3	26	-0.417	4.357	3.5
W-P	12, 14	13.5	5.111	4	3	25	-0.413	3.389	3.375

Table 1. Topological characteristics of the tested polyhedral systems

Fig.1 shows some of the traditional (periodic and space-filling) polyhedral systems. All of them are applicable to model the microstructure of polycrystalline, single-phase materials [3,10].

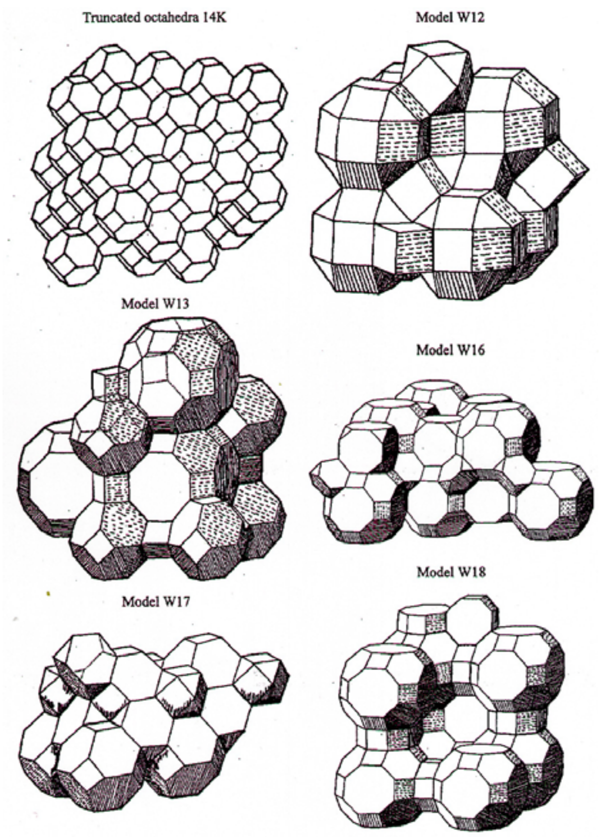

Figure 1. Examples of space-filling polyhedral systems [10]

The polyhedral system denoted by 14K represents a homogenous and regular (4-valent) cellular system, which is composed of 14-sided Kelvin polyhedra (truncated octahedra). In order to simulate the austenite transformation processes occurring in steels, the Kelvin polyhedron is widely used to the geometric modelling of the initial austenite grain structure [11]. Of the polyhedral systems shown in Fig.1, systems W17 and W18 are composed of two different polyhedra, while W12, W13 and W16 are made of three different polyhedra. In Table 1, the polyhedral system W-P is identical to the Weaire-Phelan system generated by 12- and 14-sided polyhedra. (Weaire and Phelan have recently given an example of froth with $\langle f \rangle$ =13.5 which minimize the total interfacial area [12].)

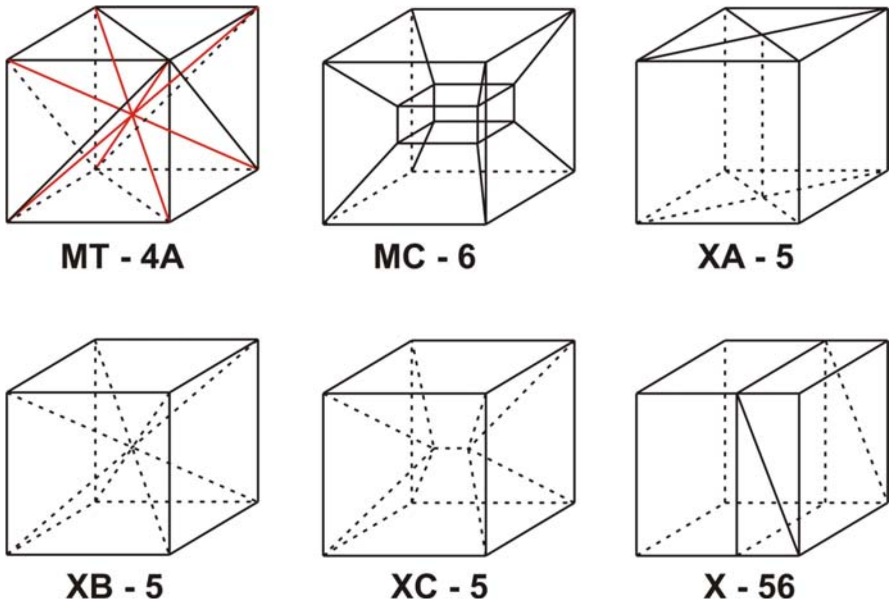

Figure 2. Artificially genereated 3-D polyhedral systems defined by their unit domains

Fig. 2 demonstrates some artificially generated space-filling periodic systems; all of them are represented by their unit domains. Of the six polyhedral systems in Fig.2, MT-4A is composed of tetrahedra, MC-6 is composed of cubes, XA-5, XB-5 and XC-5 are composed of 5-sided polyhedra. It is worth noting that the space-filling system XC-5 is constituted of topologically non-identical cells, (it is generated by two, combinatorially different 5-sided polyhedra). Relationships between the four topological shape factors are illustrated in Figs. 3-6.

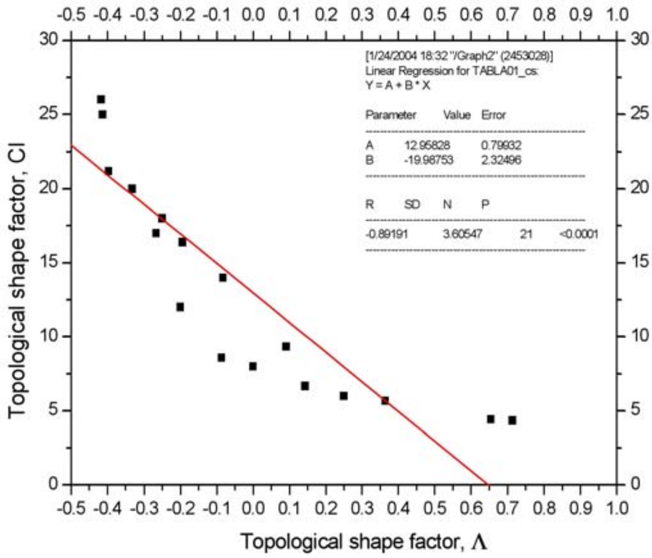

Figure 3. Relationship between topological shape factors Λ and CI

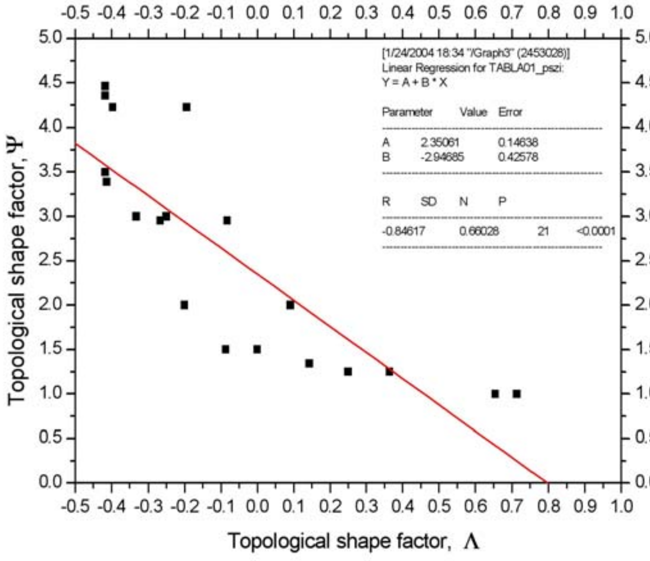

Figure 4. Relationship between topological shape factors Λ and Ψ

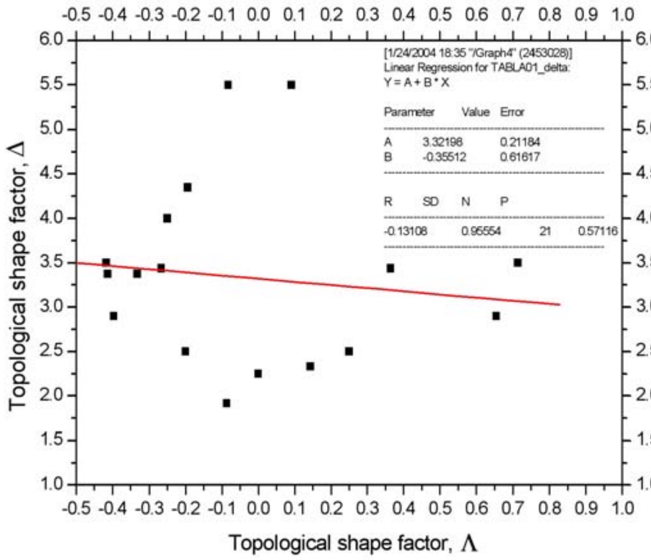

Figure 5. Relationship between topological shape factors Λ and Δ

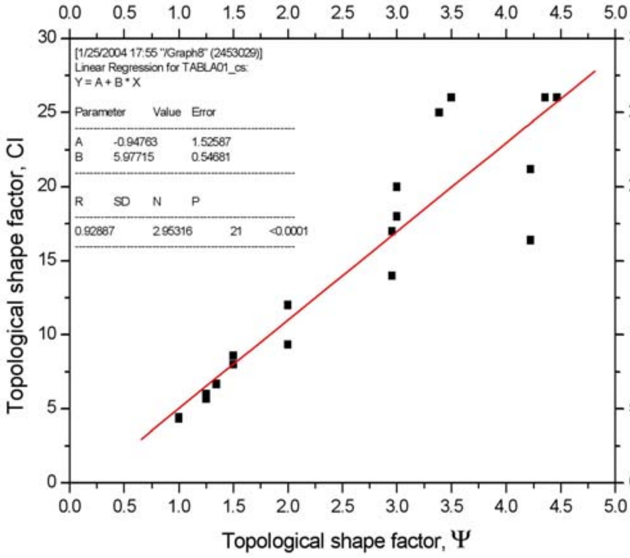

Figure 6. Relationship between topological shape factors Ψ and CI

5. Conclusions

A simple method has been developed to characterize 3-D polycrystalline microstructures modelled by space-filling polyhedral systems. From the computed results the following conclusions can be drawn:

- All of the four topological shape factors are applicable to the global geometric characterization of the simulated microstructures, although they are not algebraically independent quantities. Performing linear regression analysis and calculating the corresponding correlation coefficients R_C we have observed that there is a maximal correlation between Ψ and CI (R_C = 0.929), and a minimal correlation between Λ and Δ (R_C = - 0.131).

- Of the investigated polyhedral systems, there are three (denoted by 14K, W16 and W19) for which the values of computed topological parameters are identical, namely $\langle f\rangle$=14, [n]=36/7=5.143, [r]=4, [ε]=3, CI=26, Λ = - 0.417 and Δ=3.5. It should be noted that polyhedral systems 14K, W16 and W19 belong to the stable space-filling systems, where four polyhedra and four edges are incident on each vertex.

- Based on the concept outlined in Refs.[5,6,13], it is conjectured that for stable, periodic monotiled froths (whose cells are represented by convex polyhedra) the minimal number of faces per cell is $\langle f\rangle$=14.

- It is worth noting that in the case of the 3-D Poisson-Voronoi tessellation, the following topological quantities can be obtained:R=4, [ε]=6-12/4=3, $\langle f\rangle = 2+(48*\pi^2)/35 = 15.5355$, [n]=6-12/15.5355=5.2276, CI=29.071, Δ=Ψ=3.8839 and Λ= - 0.4261 [1]. It seems to be an open problem that the number of faces per cell $\langle f\rangle$=15.5355 can be considered as the theoretical upper bound for any stable, periodic polyhedral system whose cells are represented by convex polyhedra.

- It is important to emphasize that there exists a particular class of 3-D, 4-valent, periodic cellular structures (3-D froths), for which inequalities $\langle f\rangle$ >14, and [n] >36/7=5.143 are fulfilled. These froths are composed of "pseudo-polyhedra" (generalized polyhedra with virtual edges and vertices). An example of a stable, periodic, monotiled froth with $\langle f\rangle$ =16 and [n]=21/4 = 5.25 is given in [13]. In this case, the unit cell is a 3-valent, 16-sided pseudo-polyhedron (with the following numbers of faces: eight quadrilaterals, six hexagons and two octagons).

- It is easy to see that the proposed method can be extended to the global topological characterization of 4-dimensional polytopes which are composed of 3-D polyhedra (polyhedral cells). It can be assumed that for 4-D polytopes constituted of convex trivalent polyhedra, the upper bounds of the corresponding topological parameters are as follows: $\langle f \rangle=12$, $[n]=5$, and CI=22. The simplest 4-D polytope for which these upper bound conditions are fulfilled is the 120 cell constituted of 120 regular dodecahedra.

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