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# Correlations in topological models of 2D random cellular structures 

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#### Abstract

General relations and constraints which must be satisfied by the topological correlations in 2D space-filling random cellular structures are discussed and a topological short-range order coefficient is defined. Topological models of 2D structures are associated with planar tessellations with topologically unstable sites which belong to $z>3$ polygons. The stable configurations, called states, are obtained by replacing every vertex by $z-3$ added sides. The topological properties of the latter models are calculated exactly for a distribution of independent and equiprobable states on the various sites and for any value of $z$. The case of the structures associated with tilings by triangles is thoroughly considered. The calculated correlations are compared with the correlations in alumina cuts and in random Voronoi froths. The variability of the topological properties of 2D random cellular structures is discussed.


## 1. Introduction

The characterization of 2D random space-filling cellular structures includes in ge the distributions of metric and topological properties of single cells (cell area, lengths, cell perimeter, angles, number $n$ of edges of cells, $n_{1} \leqslant n \leqslant n_{2}$, where , in general). The two-cell correlations of metric or of topological properties have be $\epsilon_{11}$ less investigated except for $m(n)$, the mean number of edges of the first neighbour cells of $n$-sided cells ( $n$-cell). A semi-empirical law, the Aboav-Weaire law (Aboav 1970, 1980, Weaire 1974), states that $m(n)$ is linearly related to $1 / n$ by

$$
\begin{equation*}
m(n)=6-a+\left(6 a+\mu_{2}\right) / n \tag{1}
\end{equation*}
$$

where $\mu_{2}$ is the variance of the distribution $P(n)$ of the number $n$ of edges of cells: $\mu_{2}=\left\langle n^{2}\right\rangle-\langle n\rangle^{2}$, with $\langle n\rangle=6$ as consequence of Euler's relation in 2D (Weaire and Rivier 1984) and $\langle n m(n)\rangle=\mu_{2}+36$ (Weaire sum rule, Weaire 1974). In many natural random cellular structures, the parameter $a$ is of the order of 1 (Aboav 1980). If $n_{2}=\infty$, an upper limit, $a<2$, is deduced from $m(n)>4$, which holds whatever $n$ in almost all space-filling random structures (section 3). Very recently, Peshkin et al (1991) have again drawn attention to an important two-cell correlation: $M_{k}(n)$ which is the average number of $k$-sided neighbours of an $n$-cell. A similar two-cell correlation $\left(f_{n}(k)=\right.$ $\left.M_{k}(n) / n\right)$ has been theoretically considered by Lambert and Weaire (1983) for the
sake of deriving a generalization of the Weaire sum rule (section 2). $M_{k}(n)$ and $m(n)$ are related by (Peshkin et al 1991):

$$
\begin{equation*}
n m(n)=\sum_{k} k M_{k}(n) . \tag{2}
\end{equation*}
$$

Besides equation (2), the $M_{k}(n)$ must also obey the following relations (Peshkin et al 1991, see however section 3):

$$
\begin{align*}
& \sum_{k} M_{k}(n)=n  \tag{3}\\
& P(k) M_{n}(k)=P(n) M_{k}(n) . \tag{4}
\end{align*}
$$

The topological correlation functions $A_{k n}\left(A_{k n} \geqslant 0\right)$ defined as (Delannay et al 1992a):

$$
\begin{equation*}
A_{k n}=M_{k}(n) / P(k)=M_{n}(k) / P(n)=A_{n k} \tag{5}
\end{equation*}
$$

allow comparison of topological properties of tissues with different distributions $P(n)$. If the $A_{k n}$ are linear in $k$ and in $n$, they are uniquely expressed as (Delannay et al 1992a):

$$
\begin{equation*}
A_{k n}=n+k-6-\left(a / \mu_{2}\right)(n-6)(k-6) \tag{6}
\end{equation*}
$$

where $a$ is the parameter of the Aboav-Weaire law (equation (1)). Peshkin et al (1991) have applied the maximum entropy principle with constraints imposed on the distribution $P(n)$ of the number of edges of cells. They have predicted that the $M_{k}(n)$ (and consequently the $A_{k n}$ ) are linear in $n$ in order to reduce the number of independent constraints. The positivity constraint restricts the range of $a / \mu_{2}$ for which the linear relation (6) may eventually hold to $-\frac{1}{3} \leqslant a / \mu_{2} \leqslant 0$ for $n \geqslant 3$ (Delannay et al 1992a) while positive correlations among cells (few-sided cells near many-sided cells) suggest that $-\frac{1}{6} \leqslant a / \mu_{2}$ (Rivier 1993). Outside this range, distortions from linear behaviour must occur and the maximum entropy predictions must be corrected in a way which has not yet been investigated. A further source of distortion, among others, is due to the constraint $A_{33}=0$ discussed in section 3 .

The linearity of $A_{k n}$ in $k$ and in $n$ does not necessarily imply that the associated distribution $P(n)$ maximizes the entropy, $S=-\Sigma P(n) \log (P(n) / \Pi(n))$, with a prior $\Pi(n)=1$, subject to the two remaining independent constraints: $\langle 1\rangle=\Sigma P(n)=1$ and $\langle n\rangle=6$. If $\Pi(n)=1$, the maximum entropy is indeed only reached for the distribution $P_{m}(n)=0.75^{(n-3)} / 4(n \geqslant 3)$ which has very unusual features such as a mode at $n=3$ and a large $\mu_{2}=12$. More realistic distributions may be derived with appropriate prior probabilities which are unfortunately difficult to guess.

Before assessing the validity of the maximum entropy model or of any other theory devoted to random cellular structures, it is necessary to characterize in detail the topological correlations $M_{k}(n)$ or $A_{k n}$ in natural or in simulated cellular structures as well as in models. In three previous papers, we have described 2D topological models and the correlations $\boldsymbol{A}_{k n}$ in structures associated with a distribution of spins on a square lattice $(z=4)$ both for independent spins and for interacting spins (2D Ising ferromagnet as a function of temperature) (Le Caër 1991a, b, Delannay et al 1992a, referred to hereafter as I, II, III). The $A_{k n}$ correlations have been compared to experimental results published by Lewis (1931) for the epidermal epithelium of a 220 mm cucumber. A qualitative agreement and an overall fair quantitative agreement have been observed to hold between various sets of data (III).

The purpose of the present paper is to extend the exact calculation of the $A_{k n}$ to the topological models associated with any mother lattice, more particularly with
tessellations of triangles, in the case of a distribution of independent and equiprobable states (DIEs) on the lattice sites for $z$ larger than 4 (I, II). The calculated $A_{k n}$ will also be compared with correlations which have been determined in planar cuts of alumina polycrystals with some thousands of cells (Righetti et al 1992, 1993) and in a simulated Voronoi tessellation associated with a 2D Poisson point process (Stoyan et al 1987, Brakke, no publishing date). General relations and constraints on the $A_{k n}$ are first derived and discussed.

## 2. General relations and sum rules satisfied by the correlations $\boldsymbol{A}_{k n}$

Relations (2) and (3) yield

$$
\begin{equation*}
\left\langle A_{k n}\right\rangle_{n}=\sum_{k} P(k) A_{k n}=n \quad\left\langle k A_{k n}\right\rangle_{n}=n m(n) \tag{7}
\end{equation*}
$$

where the index $\langle\ldots\rangle_{n}$ means that $n$ is fixed. The correlation $A_{k n}$ can be simply expressed as a function of $P_{k n}$, the probability that a cell with $k$ sides and a cell with $n$ sides are neighbours, as

$$
\begin{equation*}
A_{k n}=6 P_{k n} /(P(k) P(n)) \tag{8}
\end{equation*}
$$

For an 'ideal' arrangement of cells free of correlations, called the topological gas, $P_{k n}$ (Fradkov et al 1987) is

$$
\begin{equation*}
P_{k n}(\text { unc. })=k n P(k) P(n) / 36 . \tag{9}
\end{equation*}
$$

The latter 'ideal' structure with trivalent vertices has cells which share two sides with some of their neighbours or one side with themselves if $P(3), P(4) \neq 0\left(P_{33}\right.$ (unc.) $\neq 0$, section 3).

Using relations (8) and (9), it is convenient to define a topological short-range order (TSRO) coefficient $\beta_{k n}=\beta_{n k}$ as
$\beta_{k n}=P_{k n} / P_{k n}($ unc. $)-1=M_{k}(n) / M_{k}(n)($ unc. $)-1=6 A_{k n} /(k n)-1$.
The TSRo coefficient is negative when $k$-cells and $n$-cells tend to repel themselves while it is positive if they tend to cluster. It is minimum and equal to -1 if $A_{k n}=0$. If the $A_{k n}$ are linear in $k$ and in $n$ (relation (6)), the TSRO coefficient $\beta_{k n}$ is given by

$$
\begin{equation*}
\beta_{k n}=-\left(1+6 a / \mu_{2}\right)(6 / k-1)(6 / n-1) \tag{11}
\end{equation*}
$$

that is $\beta_{6 n}=0$ whatever $n$ : the cells with six sides and their nearest neighbours are uncorrelated. The point $n=6$ belongs to all the hyperbola $\beta_{k n}=h_{k}(n)$. Relation (11) shows again that $a / \mu_{2} \leqslant 0$ as $\beta_{33} \geqslant-1$. Some simple general relations are derived for the $\beta_{k n}$ :

$$
\begin{align*}
& \left\langle k \beta_{k n}\right\rangle_{n}=0  \tag{12}\\
& \left\langle k^{2} \beta_{k n}\right\rangle_{n}=6\left\{m(n)-m_{\mathrm{AW}}(6)\right\} \tag{13}
\end{align*}
$$

where $m_{\mathrm{AW}}(6)=6+\mu_{2} / 6$ is the value of $m(6)$ if the Aboav-Weaire law (relation (1)) holds. Finally, a plot of $\gamma_{k n}=\beta_{k n} /(1-6 / k)(k \neq 6)$ as a function of $6 / n-1$ should give a unique straight line if relation (6) holds. Deviations from the straight line may be quantified by the correlation coefficient of a linear regression analysis.

Lambert and Weaire (1983) have generalized the Weaire sum rule $\langle n m(n)\rangle=\mu_{2}+36$. Using $\langle\langle\ldots\rangle\rangle$ to denote an average over $k$ and $n$, the Lambert-Weaire sum rule applied to the $A_{k n}$, is expressed as

$$
\begin{equation*}
\left\langle n^{q}\left\langle k^{p} A_{k n}\right\rangle_{n}\right\rangle=\left\langle n^{p}\left\langle k^{q} A_{k n}\right\rangle_{n}\right\rangle \tag{14}
\end{equation*}
$$

which is an obvious consequence of the symmetry $A_{k n}=A_{n k}$. Explicitly:

$$
\begin{equation*}
\left\langle\left\langle n^{q} k^{p} A_{k n}\right\rangle\right\rangle=\sum_{n} n^{q} P(n) \sum_{k} k^{p} P(k) A_{k n}=\sum_{k} k^{p} P(k) \sum_{n} n^{q} P(n) A_{n k} . \tag{15}
\end{equation*}
$$

Exchanging the dummy summation indices yields equation (14). The sum rule (14) is easily extended from relation (15):

$$
\begin{equation*}
\left\langle(n-6)^{q}\left\langle(k-6)^{p} A_{k n}\right\rangle_{n}\right\rangle=\left\langle(n-6)^{p}\left\langle(k-6)^{q} A_{k n}\right\rangle_{n}\right\rangle . \tag{16}
\end{equation*}
$$

Any constant may be substituted for 6 in equation (16) and negative exponents may be considered but singularities must be avoided. Relation A. 7 of Delannay et al (1992a) is simply equation (16) with $p=0$ :

$$
\begin{equation*}
\mu_{q}+1+6 \mu_{q}=\left\langle\left\langle(k-6)^{q} A_{k n}\right\rangle\right\rangle \quad \text { with } \quad \mu_{q}=\left\langle(n-6)^{q}\right\rangle \tag{17}
\end{equation*}
$$

Some nice relations are obtained, among others, for $q=-1$ and $p=0,1$ respectively:

$$
\begin{equation*}
1=\left\langle\left\langle A_{k n} / k\right\rangle_{n}\right\rangle \quad\langle m(n)\rangle=\left\langle n\left\langle A_{k n} / k\right\rangle_{n}\right\rangle . \tag{18}
\end{equation*}
$$

The general expression described in appendix A4 of III (see also Delannay et al 1993) verifies all the previous relations and sum rules:

$$
\begin{equation*}
A_{k n}=n+k-6+\sum_{i, j} c_{i j}\left[g_{i}(k) g_{j}(n)+g_{i}(n) g_{j}(k)\right] \tag{19}
\end{equation*}
$$

with $\left\langle g_{m}(k)\right\rangle=0$. Using the generalized sum rule (14), Lambert and Weaire (1983) have analysed the connection between ' $a$ ' (relation (1)) and the coefficient of kurtosis ( $\mu_{4} / \mu_{2}^{2}-3$ ) of the distribution $P(n)$.

## 3. Constraints on the repartition of cells whose vertices are trivalent

Topological characterization of the second neighbouring cells of a $n$-cell, topological constraints resulting from the condition of convexity or from the condition of vertex equilibrium, triplet correlations involving cells sharing a vertex have, to our best knowledge, not been sufficiently worked out in the literature. The present section describes some elementary but fruitful relations and conditions valid for random space-filling cellular structures with trivalent vertices. We define $m_{k}(n)$ as the number of $k$-cells which are first neighbours of an $n$-cell ( $n_{1} \leqslant n \leqslant n_{2}$ ). It is a random integer variable whose average over $n$-cells is $M_{k}(n)$. We assume that $P(3), P(4) \neq 0$.

### 3.1. Any two cells share at most one side

A cellular structure with convex cells has $A_{33}=0$ (III). This constraint also holds in any 2D structure in which each cell can at most share one side with any cell and no side with itself. Similarly, (3-cell, 4-cell, 4-cell) triplets are forbidden. Such constraints have also been considered by Godrèche et al (1992, see also Yekutieli 1992) in the enumeration of planar Feynman diagrams with a cubic interaction, which is needed to establish the properties of their topological cellular structure. The latter model is the equilibrium state which is obtained by applying repetitively a neighbour switching transformation to any initial configuration of cells with trivalent vertices.

Furthermore, any 'chain' of first neighbours of an $n$-cell, 3-4-4- . . -4-3, with a total length ranging between 3 and $n-2$, is also forbidden in such structures. Moreover, if $A_{33} \neq 0$, relation (3) is no longer strictly valid as, for instance, $\sum m_{k}(n)=n-1$ for every $n$-cell which belongs to a 3-3- $n$ triplet. Finally, the energetic cost of $A_{33} \neq 0$, which is related to the existence of a strongly concave cell, may be locally too large. The correlation $A_{33}$ is zero for our topological models ( $P_{u}(1 \mid 1, z)=0$, II and equation (24)) and there is no (3-4-4) triplet. The (3-cell, 4-cell) pair is even forbidden ( $A_{34}=0$ ) in structures associated with tilings by triangles when $z_{1}, z_{2}, z_{3} \geqslant 4$ (section 6 , figure 3 ).

### 3.2. Second neighbours

In the following, we assume that any two cells share at most one side. The second neighbours of an $n$-cell are those cells which share one side with the first neighbours of the considered cell without sharing a side with it. The total number of edges of the first neighbour cells of a given $n$-cell being $n C(n)$, the number of second neighbour cells is

$$
\begin{equation*}
s(n)=n C(n)-4 n-m_{3}(n) . \tag{20}
\end{equation*}
$$

Its average over all $n$-cells is

$$
\begin{equation*}
s_{n}=n m(n)-4 n-M_{3}(n) \tag{21}
\end{equation*}
$$

while the average number of second neighbours of a cell is

$$
\begin{equation*}
S=\left\langle s_{n}\right\rangle=\mu_{2}+12-3 P(3) \tag{22}
\end{equation*}
$$

Relation (21) has an obvious consequence: as $s_{n}$ must be positive, $m(n)$ (as well as $C(n)$ ) is larger than 4 whatever $n$. Therefore, if the Aboav-Weaire law is valid and if $n_{2}=\infty, a<2$ follows from relation 1. A simple drawing, in which a cell with any number of sides is surrounded with cells which all have four sides, shows a cellular structure in which the considered cell and its first neighbours are completely immersed in a cell without any connection with the rest of the structure.

### 3.3. Supplementary constraints

In a cellular structure with convex cells, a cell with a large number of sides cannot have too many consecutive four-sided first neighbour cells without creating second neighbour concave cells. This will increase the estimation of the minimum value of $m(\infty)$, which may become close to 5 , and will decrease the calculated upper limit of the Aboav-Weaire parameter ' $a$ '. If $s_{n}$ varies as $\Omega n$ for $n$ large, this upper limit becomes $2-\Omega$. It would be important at least to guess a reasonable value for $\Omega$. A simple solution for arranging convex cells in a way which is statistically uniform and symmetrical around very large cells, along flat boundaries or around circular boundaries, with radii much larger than the average cell size, is indeed to use almost identical five-sided cells, If the latter cells surround the central elements with two edges perpendicular (or nearly) to the boundaries, appealing pentagons with three angles equal (or close) to ( $540-180$ ) $/ 3=120^{\circ}$ can be created (mitosis of hexagons may yield such pentagons). Such a pentagon layer may constitute an efficient transition region between the boundaries and the remaining structure. Repartitions of cells which are of that type can be seen in 2D patterns of magnetic domains (Babcock and Westervelt 1989), in roots or in stems (for instance, fern or asparagus roots, pine stems, Conge 1991).

In their statistical theory of 2D grain growth, Abbruzzese et al (1992) have used a simplified model of circular grains and the assumptions of maximum and random surface covering to derive a 'special linear relationship' between $\left\langle n_{i}\right\rangle$, the average number of sides of cells with a given radius $r_{i}$ and $r_{i}\left(\left\langle n_{i}\right\rangle=3\left(1+r_{i}\right)\right)$. The same model results in a correlation, quite similar to the Aboav-Weaire law, $\left\langle m_{i}\right\rangle=$ $\left.5+\left(6+\sigma_{\langle n i}^{2}\right)\right\rangle /\left\langle n_{i}\right\rangle$, between $\left\langle m_{i}\right\rangle$, the mean number of sides of neighbours of the grain of size class $i$ and $\left\langle n_{i}\right\rangle$. The 'magic' number 5 is again retrieved.

In many cases, (3-4-n) triplets (or 3-m-3 chains of first neighbours of the $n$-cell with $m>4$ ) may raise problems of convexity at least for not too large values of $n$ and will give birth to a cell which is simultaneously separated from the $n$-cell by the 3 and 4 -cells (or by the 3 - and $m$-cells) and is a first neighbour of the $n$-cell.

Such constraints will remain valid in many structures and obviously in all structures which can be deformed into a structure with convex cells without changing the topology. It is likely that further constraints have still to be discovered.

We conclude, from the previous simple topological and geometrical arguments, that the distributions of 3 -cells and 4 -cells are correlated and that triplet correlations may also play a significant role. These correlations have not yet been fully taken into account in theoretical models. They will in general prevent the dimension of the space of constraints decreasing to two, as assumed in the maximum entropy model of Peshkin et al (1991) and will therefore lead to deviations of the $A_{k n}$ from linear behaviour. The only ' $a$ ' parameter which is consistent with the linear Maxent model in structures with $P(3) \neq 0$ and $A_{33}=0$ is strictly speaking $a=0$. The linear model may however remain a good approximation in some tissues, even for $a \neq 0$. This is the case for the topological model of Godrèche et al (1992) which displays a slight violation of the Aboav-Weaire law with $a_{w}=-\frac{6}{7}$ (appendix 3) and $\mu_{2}=10.5$.

## 4. A brief description of the topological models (I, II)

A method for constructing topological models of space-filling random cellular structures has been described in previous papers (I, II) and has been applied to two-dimensional structures. The models yield the relative repartition of cells and do not need or provide information about angles and cell-edge lengths.

We consider a lattice in which every site is characterized by its valence $z$ which is the number of edges emanating from that vertex (the fraction of vertices with $z>3$, in 2 D , being different from zero). In 2 D , every vertex, which belongs to more than $z_{s}$ $(=3)$ cells, is structurally unstable as its properties change by small deformations. The construction method is based on rules which allow removal of this unstability. The stable configuration is obtained by adding $z-3$ sides at every vertex (Thompson 1917, chapter 8 , figure $158, \mathrm{I}, \mathrm{II}$, figure 1). As the chosen rule does not create or annihilate cells, a cell of the topological cellular model is associated with every polygon of the lattice. Every added side is connected at least to one added side for $z>4$ (I and II). The latter rule produces a set of $Q(z)$ possible stable configurations, called states, which have been enumerated as a function of $z$ in II. $Q(z)$ is the Catalan number $C_{z-2}$ :

$$
\begin{equation*}
Q(z)=C_{z-2}=C_{2 z-4}^{z-2} /(z-1) \tag{23}
\end{equation*}
$$

Every state is characterized by a $z$-dimensional vector $S_{k}(k=1, \ldots, Q(z))$, whose components $S_{k j}(j=1, \ldots, z)$ have values in the range from 1 to $z-2$ (for $z=3$, $Q(3)=1$ and $S=(1,1,1)) . S_{k j}$ is the number of vertices that polygon number $j$ will
have at the considered lattice site in the final stable arrangement (figure 1). The number $n$ of sides of the cell is the sum of the $S_{k j}$ values which are inside the mother lattice polygon. The state components allows us to define the neighbours of the previous $n$-cell. Using the state components, it is unecessary to perform the transformation to the stable cellular structure in order to investigate its topological properties and full profit can be taken from the use of a periodic lattice. As the stable structure at the subject lattice site consists of $z-2$ trivalent vertices, the sum

$$
\begin{equation*}
T_{k}=\sum_{j=1}^{z} S_{k j}=3 z-6 \tag{24}
\end{equation*}
$$

is independent of the state. A configuration $\left[S_{k}\right]$ has been defined (II) as the subset of states whose components values ( $S_{k j}$ ) coincide by a circular permutation in the positive or in the negative sense of rotation (for example, the two states (1412313) and (1313214) belong to the [1231314] configuration for $z=7$, II).

An equivalent method of construction of the cellular structure uses the Euler's diagonal triangulation of the dual lattice (appendix I and figure 10 of Le Caër 1991b).

If we consider a polygon of the mother lattice with $n_{L}$ sides ( $n_{L}=3$ in figures 1 and 2), its associated cell ( $n$-cell) in the topological model has two types of neighbours (figures 1 and 2):

- unconditional neighbours which are associated with the $n_{L}$ neighbouring polygons which share one side with the considered lattice polygon
- $n-n_{L}$ conditional neighbours which are associated with the $n-n_{L}$ polygons which share one vertex with the previous lattice polygon

The values of the state components at the $n_{L}$ vertices of the mother lattice polygon provide the necessary information about the conditional neighbours.

We consider a state at a vertex of valence $z(z \geqslant 4$, figure $1(a))$ of the mother lattice and one particular component equal to $m(>1)$. If we draw a graph of the stable configuration which is associated with the previous state, the fragment of the final cell labelled by $m$ (for instance $m=3$ or 4 in figure $1(b)$ ) shares $m-1$ added sides with


(c)

Figure 1. (a) An example of a distribution of states on a triangular lattice ( $z=6$ ), the corresponding values of the number $n$ of cell sides: $n$ (large-size figures) is the sum of the state components which are inside the corresponding triangle; $(b)$ three stable states which belong to the three possible configurations for $z=6$ ([141222], [123123], [131313]); (c) one realization of a cellular structure consistent with the distribution of states of $(a)$.


Figure 2. An $n$-cell ( $n=i+j+k$ ) of the cellular structure associated with a triangle (bold lines) in the case of a tessellation of triangles (respective valences: $z_{1}, z_{2}, z_{3}$ ). The triangles which will give birth to the three unconditional neighbours and to one among the $n-3$ conditional neighbours of the $n$-cell have been indicated by Un and Co respectively. The variables $(i, s),(j, t),(k, u)$, which are state components for $z_{1}, z_{2}, z_{3}$, respectively, are used in section 6 and in appendix 1.
other fragments of cells which are parts of the conditional neighbours. It also shares two 'dangling' sides with its two immediate fragments of cells which are part of the unconditional neighbours. By extension, we call the two nearest components of a given state component its 'unconditional neighbours' (that is $S_{k j \pm 1}$ for the component $S_{k j}$, with $j+1=1$ if $j=z$ and $j-1=z$ if $j=1$ ) and the $m-1$ other components its 'conditional neighbours' (figures 11 and 12). The latter components may for instance be obtained by using the pruning algorithm described in appendix 1 of paper II.

## 5. Distributions indispensable for calculating $\boldsymbol{A}_{\text {In }}$

In order to calculate $A_{\text {ln }}$ for a dies, we must derive some distributions relative to the state components. If we write the state components as a $Q(z) \times z$ matrix, all columns contain the same set of values as required by the statistical equivalence of all $z$ polygons at any vertex: the set $S_{k j}$ for the same $j$ is the same for all $j$. We have calculated in II the number of states $n_{0}(m, z)$ (relation (4) of paper II) which have a component $m=S_{k j}(k=1, \ldots, Q(z), m=1, \ldots, z-2)$ for a fixed $j$ (which is consequently independent of $j$ ) and the corresponding distribution $P_{0}(m, z)$ :

$$
\begin{equation*}
n_{0}(m, z)=\{m /(z-2)\} \boldsymbol{C}_{2 z-5-m}^{z-3} \tag{25}
\end{equation*}
$$

with

$$
\begin{equation*}
P_{0}(m, z)=n_{0}(m, z) / Q(z)=m C_{z-1}^{m+1} / C_{2 z-4}^{m+1} \tag{26}
\end{equation*}
$$

and the average $\langle m\rangle$ is (II and relation (24))

$$
\begin{equation*}
\langle m\rangle=3(z-2) / z . \tag{27}
\end{equation*}
$$

We have also calculated the number of states $n_{u}(m \mid i, z)$ which have an unconditional component $S_{k j+1}=i$ knowing that the component $S_{k j}=m$ for a given and fixed $j$ (relation (7) of paper II):

$$
\begin{equation*}
n_{u}(m \mid i, z)=\{(i+m-2) /(z-3)\} C_{2 z-5-i-m}^{z-4} \tag{28}
\end{equation*}
$$

The corresponding distribution of the unconditional neighbours of the component $m$, is defined as

$$
\begin{equation*}
P_{u}(m \mid i, z)=n_{u}(m \mid i, z) / n_{0}(m, z) \tag{29}
\end{equation*}
$$

Without loss of generality, we consider the $n_{0}(m, z)$ states which have a first component equal to $m(m>1)$. Amongst the $(m-1) n_{0}(m, z)$ conditional neighbours (section 4) of the components equal to $m,(m-1) n_{c}(m \mid i, z)$ are equal to $i$. The factor $(m-1)$ is a consequence of the statistical equivalence of all conditional neighbours. We derive in appendix 1

$$
\begin{equation*}
n_{c}(m \mid i, z)=(i-1) n_{0}(i+m-4, z-2) \tag{30}
\end{equation*}
$$

As there are as many ( $i, m$ ) as ( $m, i$ ) pairs, the following relation:

$$
\begin{equation*}
(i-1) n_{c}(i \mid m, z)=(m-1) n_{c}(m \mid i, z) \tag{31}
\end{equation*}
$$

is obeyed as expected. The third distribution which is needed for calculating $A_{k n}$ is related to the conditional neighbours of a component ( $m \geqslant 2$ ):

$$
\begin{equation*}
P_{c}(m \mid i, z)=n_{c}(m \mid i, z) / n_{0}(m, z) \tag{32}
\end{equation*}
$$

The distributions defined by relations (26), (29), (32) will be used in the next section for calculating $P(n)$ and $A_{l n}$ for 2D cellular structures associated with tilings by triangles.

## 6. 2D cellular structures associated with tilings by triangles

### 6.1. Theoretical expressions for $P(n)$ and $A_{l n}$

We will only consider tilings in which the vertices of every triangle have respective valences $z_{1}, z_{2}, z_{3}$. As shown by figure 2 , the number of sides $n$ of the cell associated with the bold triangle is a random variable which is the sum of three independent random variables (DIEs) $i, j, k$ with

$$
\begin{array}{lcc}
Z_{s}=z_{1}+z_{2}+z_{3} & 3 \leqslant n \leqslant Z_{s}-6 & \\
1 \leqslant i \leqslant z_{1}-2 & 1 \leqslant j \leqslant z_{2}-2 & 1 \leqslant k \leqslant z_{3}-2 . \tag{34}
\end{array}
$$

As $\langle n\rangle=\langle i\rangle+\langle j\rangle+\langle k\rangle=6$ (Euler's relation), the valences $z_{1}, z_{2}, z_{3}$ must satisfy the following condition (relation (27)):

$$
\begin{equation*}
\sum_{m=1}^{3}\left(z_{m}-2\right) / z_{m}=2 \tag{35}
\end{equation*}
$$

which has also been derived in various ways by Grünbaum and Shephard (1987). The distribution of the number of edges of cells $P(n)$ is given by

$$
\begin{equation*}
P(n)=\sum_{i=1}^{z_{1}-2} \sum_{j=1}^{z_{2}-2} \sum_{k=1}^{z_{3}-2} \partial(n-i-j-k) P_{R 3}(i, j, k) \tag{36}
\end{equation*}
$$

with

$$
\begin{equation*}
P_{R 3}(i, j, k)=P_{0}\left(i, z_{1}\right) P_{0}\left(j, z_{2}\right) P_{0}\left(k, z_{3}\right) . \tag{37}
\end{equation*}
$$

Some values of $P(n)$ and of $n m(n)$ for particular values of $n$ are given in appendix 2. As $i, j, k$ are independent variables, the variance $\mu_{2}$ of the distribution $P(n)$ is simply derived from equation A2.1 of paper II:

$$
\begin{equation*}
\mu_{2}=\sum_{m=1}^{3} 2\left(z_{m}-2\right)\left(z_{m}-3\right)\left(2 z_{m}-3\right) /\left\{z_{m}^{2}\left(z_{m}+1\right)\right\} \tag{38}
\end{equation*}
$$

Equations (36) and (38) are easily generalized for a DIES on the vertices of any tiling. With the help of figure 2, it is simple to deduce

$$
\begin{equation*}
A_{t n}=\left\{\sum_{\substack{i, j, k \\ s, r, u}} \partial(n-i-j-k) \partial(l-s-t-u) P_{R 3}(i, j, k) F(i, j, k, s, t, u)\right\} /[P(l) P(n)] \tag{39}
\end{equation*}
$$

where $(i, s),(j, t),(k, u)$ range from 1 to $z_{1}-2, z_{2}-2, z_{3}-2$, respectively, and $F(i, j, k, s, t, u)$ is a sum over the unconditional and conditional neighbours (figure 2). Defining

$$
\begin{equation*}
P_{R u}(i, s, j, t)=P_{u}\left(i \mid s, z_{1}\right) P_{u}\left(j \mid t, z_{2}\right) \tag{40}
\end{equation*}
$$

and

$$
\begin{equation*}
P_{R 0}(s, t)=P_{0}\left(s, z_{1}\right) P_{0}\left(t, z_{2}\right) \tag{41}
\end{equation*}
$$

(and similarly for all combination of variables). We finally write
$F(i, j, k, s, t, u)$

$$
\begin{align*}
= & P_{R u}(i, s, j, t) P_{0}\left(u, z_{3}\right)+P_{R u}(i, s, k, u) P_{0}\left(t, z_{2}\right) \\
& +P_{R u}(j, t, k, u) P_{0}\left(s, z_{1}\right)+(i-1) P_{c}\left(i \mid s, z_{1}\right) P_{R 0}(t, u) \\
& +(j-1) P_{c}\left(j \mid t, z_{2}\right) P_{R 0}(s, u)+(k-1) P_{c}\left(k \mid u, z_{3}\right) P_{R 0}(s, t) . \tag{42}
\end{align*}
$$

From the definitions of $P_{0}, P_{u}$ and $P_{c}$ (section 5) as well as from relation (31), it is readily shown that $A_{\text {in }}=A_{n t}$. Relations (36) and (39) have been used in a microcomputer Fortran program to calculate $P(n)$ and $A_{i n}$ in double precision, with an absolute error less than $10^{-12}$, for any possible combination of $z_{1}, z_{2}, z_{3}$. Exact values have been calculated for $z_{1}=z_{2}=z_{3}=6$ (Mathematica would yield exact values in all cases). Relation (39) gives the expected correlation $A_{33}=0$ (section 3) as $A_{33}$ is uniquely obtained for $i=j=k=s=t=u=1$ and $F(1,1,1,1,1,1)=0$. Finally, $P(n)$ is very well approximated by the generalized Poisson distribution (Consul 1989) for $\mu_{2} \geqslant 3$ (relation (44)).

### 6.2. Results

There are ten triplets $\left(z_{1}, z_{2}, z_{3}\right)$ which verify relation (35) (table 1 , Grünbaum and Shephard 1987). All the numerical calculations have been checked with the help of relations (7) and (A2.5)-(A2.8). However, for the six triplets indicated by a star in table 1 , it is not possible to extend the neighbourhood of a starting vertex to a tiling of the plane (Grünbaum and Shephard 1987, chapter 2).

The $P(n)$ and $A_{l n}$ calculated with the relations of section 6.1 for the six 'pathological' triplets verify nevertheless all conditions which must be fulfilled by these quantities

Table 1. Some characteristics of the 2 D cellular structures associated with tilings by triangles (except $z=4$ for the square lattice and $z=5$ for a tiling by squares and triangles, I, II) sorted in order of increasing $\mu_{2}$, the variance of $P(n) z_{e}$ is an effective valence calculated from relations (A2.3) and (A2.4); $a_{w}$ is the Aboav-Weaire parameter calculated from relation (A3.1); the asterisk indicate triplets, which verify condition (35), for which a tiling of the plane does not exist).

| $z_{1}-z_{2}-z_{3}$ | $z_{e}$ | $\mu_{2}$ | $a_{w}$ | $P(6)$ |
| :---: | :---: | :---: | :---: | :---: |
| $4$ <br> (squ) | 4 | 1 | 1.5 | 0.375 |
| 6-6-6 | 6 | $\begin{aligned} & 18 / 7 \\ & (2.57143) \end{aligned}$ | 1 | 0.236880 |
| $\begin{aligned} & 5 \\ & (\mathrm{squ}+\mathrm{Tr}) \end{aligned}$ | 5.38 | $\begin{aligned} & 194 / 75 \\ & (2.58667) \end{aligned}$ | 1.212618 | 0.238934 |
| 5-5-10* | 6.783 | $\begin{aligned} & 784 / 275 \\ & (2.85091) \end{aligned}$ | 0.725510 | 0.228923 |
| 4-8-8 | 6.775 | $\begin{aligned} & 71 / 24 \\ & (2.95833) \end{aligned}$ | 0.721831 | 0.219353 |
| 4-6-12 | 7.542 | $\begin{aligned} & 569 / 182 \\ & (3.12637) \end{aligned}$ | 0.532514 | 0.218321 |
| 4-5-20* | 10.134 | $\begin{aligned} & 1227 / 350 \\ & (3.50571) \end{aligned}$ | 0.142439 | 0.212208 |
| 3-12-12 | 9.354 | $\begin{aligned} & 105 / 26 \\ & (4.03846) \end{aligned}$ | 0.214286 | 0.187306 |
| 3-10-15* | 9.721 | $\begin{aligned} & 2239 / 550 \\ & (4.07091) \end{aligned}$ | 0.176838 | 0.187244 |
| 3-9-18* | 10.450 | $\begin{aligned} & 706 / 171 \\ & (4.12865) \end{aligned}$ | 0.110997 | 0.187115 |
| 3-8-24* | 12.250 | $\begin{aligned} & 509 / 120 \\ & (4.24167) \end{aligned}$ | -0.015037 | 0.186794 |
| 3-7-42* | 18.234 | $\begin{aligned} & 9385 / 2107 \\ & (4.45420) \end{aligned}$ | $-0.242860$ | 0.185914 |

(introduction). This stems in part from the fact that the averaging procedure which is performed on all states in the calculation of both $P(n)$ and $A_{l n}$ decouples the successive $z_{p}(p=1,2,3)$ sectors at the vertices which contribute to $P_{0}\left(s, z_{1}\right)$ and $P_{R 0}(s, t)$, etc, in the first three terms and in the last three terms of equation (42) respectively (figure 2). It is therefore possible to calculate all the previous properties without knowing how to construct the associated cellular structure. We have not been able to prove if a given set of $P(n)$ and $A_{l n}$ which fulfils all constraints suffices to define a cellular structure with such topological properties or if extra conditions are required. The 'pathological' results have nevertheless been included in the following analysis. Appendix 3 further describes a set of $P(n)$ and $A_{l n}$, valid for $n, l \geqslant 4$, which yields the Aboav-Weaire law with $a=-1$.

Some correlations have been plotted in figure 3: the trend towards an increase of $A_{l n}$ with $l$ for small $n$ is progressively transformed into a trend towards a decrease for large $n$. Figure $3(a)$ moreover shows the curvature due to the positivity constraint for large $l$ and $n$. The Aboav-Weaire parameter $a_{W}$ decreases with $\mu_{2}$ (table 1) and becomes negative for large values of $\mu_{2}$. The topological structures considered by Peshkin et al (1991) and by Godrèche et al (1992) also show negative values of ' $a$ ', close to -1 , for $\mu_{2} \approx 10$. Empirical relationships describe with a good accuracy the dependence of $a_{w}$ and of $a_{w} / \mu_{2}$ on an effective valence $z_{e}$ defined by relations A2.3 and A2.4


Figure 3. Correlations $A_{l n}$ for cellular structures associated with tilings by triangles: (a) $z_{1}=3, z_{2}=12, z_{3}=12$ (DIES, $3 \leqslant l, n \leqslant n_{2}=21, A_{34} \neq 0$ ); (b) $z_{1}=4, z_{2}=6, z_{3}=12$ (Dies, $3 \leqslant l, n \leqslant n_{2}=16, A_{34}=0$ ). In both cases $l$ decreases from top to bottom in the left part ( $n=4$ ) while it tends to increase in the right part ( $n=n_{2}$ ).


Figure 4. The Aboav-Weaire parameter $a_{w}$ (full circles) and $a_{w} / \mu_{2}$ (open circles) as a function of the effective valence $z_{e}$ (appendix 2) for the cellular structures of table 1 . The full lines are calculated from $\left(a_{w}=-0.52+4.663 /\left(z_{e}-3\right), z_{e} \geqslant 6\right)$ and from $\left(\alpha_{w} / \mu_{2}=-0.196+1.683 /\left(z_{e}-3\right), z_{e} \geqslant 4\right)$.


Figure 5. Mean total number of sides $n m(n)$ of the first neighbour cells of $n$-cells for a DIES on the vertices of a 3-12-12 tiling. The straight line is obtained from a fit in the range 3-10.
(appendix 2) (figure 4) and the dependence of $a_{w}$ on $\mu_{2}$ :

$$
\begin{equation*}
a_{w}=-1.486+6.341 / \mu_{2} \quad \text { for } \mu_{2} \geqslant 2.5 \tag{43}
\end{equation*}
$$

Figure 5 shows $n m(n)$ for a cellular structure associated with a dies on the vertices of a 3-12-12 tiling. The straight line of figure 5 suggests that an Aboav-Weaire law with $a=0.175 \pm 0.010$, close to $a_{w}=0.2143$ (table 1), holds for a limited range of $n$ ( $3 \leqslant n \leqslant 10$ ). The Aboav-Weaire law is never rigorously verified in the structures associated with tilings by trangles but $n m(n)$ departs often not so much from linearity for $n$ ranging from 3 to $\approx 10$. The curvature of $n m(n)$ is clearly seen for large $n$ values which are not usually accessible in typical experiments. Extrapolation of the $n m(n)$ behaviour observed in a restricted range of $n$ must be performed with care.

## 7. Comparison of topological models with natural or artificial structures

### 7.1. Alumina cuts

As already emphasized (II), the distributions $P(n)$ of structures associated with a DIES on the vertices of any tessellation with $z \geqslant 5$ are typical of the $P(n)$ of planar cuts of polycrystals and differ from the $P(n)$ of soap froths. The topological and the metric properties of planar cuts of polycrystals, showing about 7000 grains, have been recently characterized by Righetti et al (1992, 1993). We have used the latter data to calculate $A_{k n}$ from the 4310 most central grains. As $a_{w}=1.19$ and $\mu_{2}=2.585$ for the polycrystal cut, we have chosen to compare its $\boldsymbol{A}_{k n}$ correlations with the correlations in a structure associated with a dies on the pentavalent vertices of a tessellation of squares and triangles (figure 1 of reference II) with $a_{w}=1.2126$ and $\mu_{2}=2.5867$. The distribution $P(n), n m(n)$ (figure 6) as well as $A_{k n}$ (figure 7) are quite similar.

### 7.2. Random Voronoi froth

The Voronoi tessellation (RVF) associated with a 2D poisson process has been investigated by various authors. Using the simulation results of Brakke (report without publishing date) with more than two hundred million cells, we calculate $a_{w}=0.6471$


Figure 6. Distributions $P(n)$ and $n m(n)$ of alumina planar cuts (open circles, Righetti et al 1993) and of a structure corresponding to a DIES on a $z=5$ lattice (fuil triangles, II).
while $\mu_{2}=1.7807 \pm 0.0004$, that is $a_{w} / \mu_{2}=0.3634$. The cellular structure associated with a dies on the vertices of a triangular lattice has different values of $a_{w}(=1)$ and $\mu_{2}$ ( $=2.5714$, table 1) but a similar $a_{w} / \mu_{2}$ ratio ( $=0.3889$ ). Figure 8 shows the strong similarities between the two sets of correlations $A_{k n}$ and of rsRo coefficients $\beta_{k n}$ in the common $k, n$ ranges while the $P(n)$ (figure 9) and $n m(n)$ are definitely different. We also notice that the correlations $\boldsymbol{A}_{k n}$ (or $\beta_{k n}$ ) are rather close in the previous alumina cuts and in the RVF.

The tsro coefficients show that cells with less than six sides tend to avoid neighbouring cells with less than six sides while they tend to attract cells which have more than six sides. The reverse holds for cells with more than six sides. The TSRO $\beta_{6 n}$ are almost equal to zero for the RVF and for $z=6$. The strongest deviations between the two sets of TSRO coefficients (figure 8) occur either for $n=3$ or for $n$ larger than $\approx 9$. This is also true for the models of the present work, for structures with very different $\mu_{2}$. More generally, we observe a restricted variability of topological properties of different structures with similar values of $\mu_{2}$. The topological correlations are, for instance, quite similar in structures with $\mu_{2} \approx 1$ such as biological tissues, Ising model, tessellations associated with 2D hard-disk packings, computer simulations including mitosis (Delannay et al 1992a, Mombach et al 1992). No comparison with the topological correlations of soap froths can be performed as such data are not available. The 'inescapable mathematical requirements of space-filling' (Smith 1954, Rivier 1985, 1986, 1993), as well as the conditions (section 3) imposed by cell shapes which depart


Figure 7. Correlations $A_{k n}$ for alumina cuts (full circles, open and full squares) and for a DIES on a $z=5$ lattice (full lines) for $3 \leqslant k, n \leqslant 10$.
in general not too much from some kind of regularity, strongly constrain 2D random cellular structures and restrict the accessible ranges of properties.

## 8. Universal $\mu_{2}=f(P(6))$ relation

In recent papers, Lemaître et al $(1992,1993)$ and Gervois et al (1992) have shown that the second moment $\mu_{2}$ of the distribution $P(n)$ of the number of cell edges varies quasi-universally with the fraction $P(6)$ of six-sided cells. According to Lemaitre et al (1992b) the relation between $\mu_{2}$ and $P(6)$ is the equivalent in random mosaics of the virial equation of state in statistical mechanics. Gervois et al (1992) have investigated the 20 mosaïcs obtained by a Voronoi tessellation of a monosize assembly of disks at different packing fractions. Applying the maximum entropy principle with the constraints $\langle 1\rangle=1,\langle n\rangle=6,\left\langle f_{n}\right\rangle=\langle 1 / n\rangle=$ constant, they have been able to derive a theoretical $\mu_{2}=f(P(6))$ relationship which is in good agreement with experiment. Gervois et


Figure 8. (a) Correlations $A_{k n}$; (b) Topological short-range order coefficients $\beta_{k n}$ : for a random Voronoi froth (RVF) and for a DIES on a $z=6$ lattice (full lines) for $3 \leqslant k \leqslant 11$, $3 \leqslant n \leqslant 15$. For the RVF, the correlations have been calculated from the incidence matrix given by Brakke. For every figure, the full circles correspond to the smallest value of $k$, the open squares to the intermediate value of $k$ and the full squares to the largest value of $k$.
al (1992), however, emphasize that the calculated results are not very sensitive to the choice of $f_{n}$ (power law, logarithm or exponential law). Figure 10 shows an extended plot of results available from biology, metallurgy, hard-disk experiments and simulations, soap froths and from various models and computer simulations. Le Caër (1991b) has also observed that the topological defect concentration $C=3 P(3)+4 P(4)+5 P(5)$ plotted for a number of cellular structures as a function of $\mu_{2}$ clusters in a narrow region of the ( $C, \mu_{2}$ ) plane. No structure, amongst the structures considered in figure 10 , seems to deviate significantly from the overall behaviour. Besides the Voronoi froths for which 'the essential physics has been lost' (Rivier 1993), these structures include the 'pathological' structures of table 1 and even some distributions $P(n)$ for which it is not proven that they can be associated with any actual cellular structure


Figure 9. Distributions $P(n)$ for a random Voronoi froth (full circles, Brakke) and for a DIES on a $z=6$ lattice (open circles).
(see also below). This strongly suggests to ascribe part of the quasi-universal behaviour to the strong constraints which act on such structures. As discussed by Le Caër (1991b) for $C$, a rather narrow range of $P(6)$ and of $C$ may be only available as a consequence of $\langle n\rangle=6$ for $n \geqslant 3$ and a given $\mu_{2}$ if moreover the $P(n)$ distributions must be 'smooth' and 'unimodal' (although the distributions are discrete). The preceding arguments are reinforced by considering various families of discrete probability distributions which depend on two parameters at least. One relation between the parameters enables us to fix the mean $\langle n\rangle=6$ while the extra degrees of freedom allow varying $\mu_{2}$. The generalized Poisson distribution and the negative binomial distribution (Consul 1989) are examples of such families. The generalized Poisson distribution with a parameter $\lambda$, that we restrict here to $3 \geqslant \lambda \geqslant 0$, with $\langle n\rangle=6, n \geqslant 3$ and $\mu_{2}=27 / \lambda^{2}$ is
$P(n)=\lambda\{\lambda+(n-3)(1-\lambda / 3)\}^{(n-4)} \exp [-\lambda-(n-3)(1-\lambda / 3)] /(n-3)!$.
The product $\mu_{2}^{0.5} P(6)=4.5 \mathrm{e}^{-3} \sqrt{3} \approx 0.38805$ is independent of $\lambda$. When $P(6)$ ranges from $\approx 0.7$ to $\approx 0.1$, the relation $\mu_{2}^{\alpha} P(6)=\delta$, with $\alpha=0.54096,0.5492$ and $\delta=0.40935$, 0.39414 , is a very good approximation of the theoretical values for the negative binomial distribution and the Maxent distribution (figure 10), respectively. For the Voronoi tessellations associated with monosize disk assemblies on an air cushion table (Lemaître et al 1993), we obtain a good agreement with experiment for $\alpha=0.513$ and $\delta=0.398$. The reduced variability of $\alpha$ and $\delta$ suggests to fit the data of figure 10 with the latter power law. We derive thus a useful approximate relation

$$
\begin{equation*}
\mu_{2}^{0.513} P(6)=0.3893 \quad \text { for } 0.7 \geqslant P(6) \geqslant 0.1 \tag{45}
\end{equation*}
$$

which yields calculated values of $P(6)$ with a precision in general better than $5 \%$ and at worst better than $\approx 10 \%$. Relation (45) predicts $P(6)=0.679,0.4332,0.3177,0.2896$, 0.1165 instead of $P(6)=0.682,0.415,0.305,0.2947,0.1168$, for a packing of disks with $\mu_{2}=0.338$ (Lemaître et al 1993), and epidermal epithelium of a 220 mm cucumber (Lewis 1931, $\mu_{2}=0.812$ ), a 2D soap froth (Glazier 1989, $\mu_{2}=1.486$ ), the random Voronoi froth ( $\mu_{2}=1.7807$ ) and the model of Godrèche et al ( $1992 \mu_{2}=10.5$ ) respectively. A still satisfactory relation, that is easier to remind, is $\mu_{2} P(6)^{2}=0.150( \pm 0.014)$. Finally, the preceding discussion is also in agreement with the reduced variability of the topological properties which has been observed in section 7.


Figure 10. $\mu_{2}=f(P(6))$ for various 2D cellular structures. Full lines in (a) and (b) are calculated by the Maxent method with the constraints $\langle 1\rangle=1,\langle n\rangle=6,\left\langle(n-6)^{2}\right\rangle=\mu_{2}$ (given). Besides the points ( $\mu_{2}, P(6)$ ) already plotted by Lemaître et al (1992, 1993 and references therein) or the points taken from the compilation of Glazier (1989), some noteworthy points are: ( $a$ ) the largest $\mu_{2}$ value (full circle, Carnal and Mocellin 1981, $\mu_{2}=16.4$ ), the upper open circle (Godrèche et al 1992, $\mu_{2}=10.5$ ), the other open circles which correspond to structures with two-sided cells (Le Caër 1991b, $\mu_{2}=8$ ) and to 20 Johnson-Mehl froths (Frost and Thompson 1987); (b) all the points given in table 1 of the present work (full triangles), the open triangles associated with the RVF (Brakke) and with alumina cuts (Righetti et al 1993), the full circles (Carnal and Mocellin 1981); (c) the crosses obtained from hard-disk simulations (Fraser et al 1990 and personal communication), the full (air table) and open (random sequential absorption) squares results of Lemaître et al (1992, 1993), the upper and lower full lines are for the topological models on a square lattice for independent and Ising distributions of spins respectively (Le Caër 1991a, Delannay et al 1992b).

## 9. Conclusion

Constraints on the topological correlations in a number of cellular structures have been discussed and a topological short-range order coefficient has been defined. We have derived all the distributions which allow exact calculation of the properties of the topological models associated with a distribution of independent and equiprobable states on the vertices of any mother tiling. These properties have been investigated in detail for the case of a dies on the vertices of tilings by triangles. The topological correlations confirm that the dies structures are typical of the experimental properties of polycrystal cuts.

The natural structures and the artificial structures, with comparable $\mu_{2}$ values, which have been considered here and in a previous paper (Delannay et al 1992a) exhibit similar topological properties when $n$ ranges between $\approx 4$ and $\approx 10$. More generally, the toplogical properties seem to vary smoothly when $\mu_{2}$ increases. The strong constraints acting on 2D random structures may suffice to explain the fair quantitative agreement which exists between the topological properties of various cellular structures and the properties of our models which include no physics but already take into account many of the most important constraints. The restricted variation of properties is a source of confusion which makes it difficult to sort the assumptions of a given theory which are actually confirmed by experiment. Although our models prevent us by nature to question the validity of any 'reasonable' physical theory, they call for a finer theoretical as well as experimental discrimination of the topology of 2 D random cellular structures.

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## Appendix 1. Enumeration of the unconditional neighbours of a component $\boldsymbol{m}$

Amonst the $Q(z)$ trees associated with a given valence $z(z \geqslant 5$, II, section 4, figure 1), $n_{0}(m, z)$ have a first component equal to $m(1 \leqslant m \leqslant z-2)$. In order to calculate $n_{c}(m \mid i, z)$ (section 6, relation (30)), we will define a new operation, which does not reduce in general to a single neighbour switching (Weaire and Rivier 1984, figure 9 of II). It consists in joining the two dangling sides shared between the component $m$ and its two unconditional neighbours (figure 11(a)), and in cutting one of the edges of the cycle created by the joining operation (figure $11(b)$ and (c)).

This joining-cutting operation is illustrated in figure 11 and symbolized in figure 12 for $z=8$, the state (41313312) and $m=4$. We define a systematic and unambiguous way of performing the cutting operation. For that purpose, we write the state components on a circle, in an anticlockwise positive sense of rotation (figure 12) starting


Figure 11. A joining and cutting operation performed on a (41313312) state for $z=8$. The bold lines in $A$ are joined as shown in $B, C$ is rotated with respect to $B$ for a more convenient reading. The bold hatched line in $B$ is cut to give the final state (42133131) in $C$. The circled component $m$ is the first state component in $A$ and $C$. The components in squares are the unconditional neighbours of $m$ in the initial state and a conditional neighbour of $m$ in the final state while the reverse holds for the components in diamonds.


Figure 12. A symbolic representation of the joining and cutting operation of figure 11. The component in diamond in $A$ is the last conditional neighbour of $m=4$. The thin lines connect the $m$ component to its two unconditional neighbours $u_{1}=1$ and $u_{2}=2$ (components in squares). The bold lines connect $m$ to its conditional neighbours ( $m-1$ lines).
with the component $m$ (circled number). The conditional neighbours are sorted according to their position along the circle, starting from $m$ in the positive direction. We systematically cut the side of the cycle shared between the $m$ component and its last conditional neighbour $c$ (figures 11 and $12, c=3$ ). The joining-cutting operation so defined is identical with the following set of operations ( $1,2,3$ ) on the state components (figures 11 and 12)
(i) Consider the state $\left(m, u_{1}, \ldots, c, \ldots, u_{2}\right)$. The last conditional neighbour of $m$ is $c$.

1. Sum up $u_{1}$ and $u_{2}: u=u_{1}+u_{2}$.
2. Split $c$ in two: $c=c_{1}+c_{2}, c_{1}$ and $c_{2}$ being the total number of neighbours of $c$ located between $c$ and $m$ and between $m$ and $c$ respectively ( $m$ is not taken into account).
3. Suppress $m$, replace $u_{1}$ by $u$, suppress $u_{2}$, replace $c$ by the sequence $c_{2}, m, c_{1}$.
(e) Rewrite the state components in the positive sense with $m$ as the first component ( $m, c_{1}, \ldots, u, \ldots, c_{2}$ ).

Figure 12 gives an example of the joining-cutting operation performed on the state ( 41313312 ) with $m=4, c=3, u=1+2, c_{1}=2$ and $c_{2}=1$ for $z=8$ which is transformed into ( 33131421 ) which finally gives (42133131). The same operation performed on ( 42133131 ) gives back the initial state. These two states belong to a cycle of length 2.

For $z=8$ and $m=4, n_{0}(4,8)=14$, three cycles of length 4 are obtained besides the latter cycle.

The initial state and the final str $e$ are in a one-to-one correspondence. In general the subset of states with a first component equal to $m$ is split into cycles of a smaller number of trees which are globally left invariant by the transformation. In the final state obtained after cutting, we know that $u$ is a conditional neighbour of $m$. The number of states which have a sequence $u_{1} m u_{2}$ for a given $m$ in a fixed position is (relation A2.3 of Le Caër 1991b after correcting a typing error: $2 z-5$ replaces $2 z+5$ ):

$$
\begin{equation*}
n\left(u_{1}|m| u_{2}\right)=\left\{\left(u_{1}+u_{2}+m-4\right) /(z-4)\right\} C_{2 z-5-u_{1}-u_{2}-m}^{z-5} \tag{A1.1}
\end{equation*}
$$

for $m>1$. The number $n_{c}(m \mid i, z)$ is therefore given by

$$
\begin{align*}
n_{c}(m \mid i, z) & =\sum_{k=1}^{i-1} n(i-k|m| k)=(i-1)\{(i+m-4) /(z-4)\} C_{2 z-5-i-m}^{z-5} \\
& =(i-1) n_{0}(i+m-4, z-2) \tag{A1.2}
\end{align*}
$$

The factor ( $i-1$ ) is simply related to the fact that an $i=1$ component has no conditional neighbour. The average of $P_{u}(m \mid i, z)$ (relation (29)) has been calculated in II:

$$
\begin{equation*}
\left\langle i_{u}(m, z)\right\rangle=[(m+1) / m]\{(2 z-m-4) /(z-1)\} . \tag{A1.3}
\end{equation*}
$$

The average of $P_{c}(m \mid i, z)\left(=n_{c}(m \mid i, z) / n_{0}(m, z)\right)$ is

$$
\begin{equation*}
\left\langle i_{c}(m, z)\right\rangle=2\left\langle i_{u}(m, z)\right\rangle \tag{A1.4}
\end{equation*}
$$

which is expected on the basis of the statistical equivalence of all fragments of cells around the central cell after joining (figure $11(b)$ ). Relations (A1.3) and (A1.4) explain relation (Al.2) of paper II.

## Appendix 2. Convenient relations for tilings by triangles

Some values of $P(n)$ are directly calculated for a dies on the vertices of a tiling by triangles (the vertices of every triangle have respective valences $z_{1}, z_{2}, z_{3}$, $Z_{s}=z_{1}+z_{2}+z_{3}$ ):

$$
\begin{array}{cc}
P(3)=\prod_{m=1}^{3}\left[Q\left(z_{m}-1\right) / Q\left(z_{m}\right)\right] & P(4)=3 P(3) \\
P\left(Z_{s}-6\right)=\prod_{m=1}^{3}\left[1 / Q\left(z_{m}\right)\right] & P\left(Z_{s}-7\right)=\left(Z_{s}-9\right) P\left(Z_{s}-6\right) \tag{A2.2}
\end{array}
$$

To a given triplet $\left(z_{1}, z_{2}, z_{3}\right)$, we associate an effective valence $z_{\varepsilon}$ defined as

$$
\begin{equation*}
Q_{a}\left(z_{c}\right)^{3}=Q\left(z_{1}\right) Q\left(z_{2}\right) Q\left(z_{3}\right) \tag{A2.3}
\end{equation*}
$$

where $z_{e}$ is in general not an integer. $Q_{a}(z)$ is a high precision approximation to $Q(z)$ $Q_{a}(z)=4^{2} \exp \left\{-1 /[8(z-2)]+1 /\left[192(z-2)^{3}\right]\right\} /\left\{16 \pi^{1 / 2}(z-1)(z-2)^{1 / 2}\right\}$.
A direct and straightforward calculation yields values of $n m(n)$ (section 1), for $n=3$, $4, Z_{s}-6$, which are useful for checking the valdity of the calculation of $A_{\text {ln }}$ (relation (39))

$$
\begin{equation*}
3 m(3)=6+4 \sum_{i=1}^{3}\left(2 z_{i}-5\right) /\left(z_{i}-1\right) \tag{A2.5}
\end{equation*}
$$

as well as

$$
\begin{array}{ll}
4 m(4)=10+\frac{4}{3} \sum_{i=1}^{3}\left(7 z_{i}-19\right) /\left(z_{i}-1\right) & \text { if all } z_{i}>3 \\
4 m(4)=10.5+2 \sum_{i=1}^{3}\left(5 z_{i}-14\right) /\left(z_{i}-1\right) & \text { if one } z_{i}=3 \tag{A2.7}
\end{array}
$$

and

$$
\begin{equation*}
\left(Z_{s}-6\right) m\left(Z_{s}-6\right)=5 Z_{s}-24 \tag{A2.8}
\end{equation*}
$$

when $Z_{s} \rightarrow \infty, m\left(Z_{s}-6\right) \rightarrow 5$, a limit very often found and discussed (Peshkin et al 1991, section 3 ).

## Appendix 3. Concerning the Aboav-Weaire law

## An Aboav-Weaire parameter for nonlinear $n m(n)$

When $n m(n)$ is not linear in $n$, it is easy and convenient (III) to calculate ' $a$ ' (equation (1)) from a weighted least-squares fit of $n m(n)$ with weights $W_{n}=P(n)$. The latter fit has the unique feature to provide a single parameter $a_{w}$ from a linear fitting of $n m(n)$ :

$$
\begin{equation*}
a_{w}=\left(216+12 \mu_{2}-\left\langle n^{2} m(n)\right\rangle\right) / \mu_{2} \tag{A3.1}
\end{equation*}
$$

The average $\langle n\rangle$ and $\langle n m(n)\rangle$ may differ from 6 and $\left\langle n^{2}\right\rangle$ respectively for a finite network on a plane. Relations (1) and (A3.1) are replaced in that case respectively by

$$
\begin{align*}
& m(n)=\langle n\rangle-a+\left(\langle n m(n)\rangle-\langle n\rangle^{2}+a\langle n\rangle\right) / n  \tag{A3.2}\\
& a_{w}=\left(\langle n\rangle\left\langle\langle n m(n)\rangle+\mu_{2}\right\}-\left\langle n^{2}(m(n)\rangle\right) / \mu_{2} .\right. \tag{A3.3}
\end{align*}
$$

## Nonlinear correlations which yield the Aboav-Weaire law

Le Caër (1991b) has considered a spherical tessellation which consists of $z$ half great circles which share two poles and includes an equatorial circle. A z-3-3-3 tessellation is obtained if the half great circles are regularly spaced and if one hemisphere is rotated with respect to the second one by half of the spacing. The following relations also hold for the corresponding planar tessellation (II) but only in the limit of large $z$. The distribution $P(n)$ is given by $P_{0}(n-3, z)$ while the $A_{k n}$ are
$A_{k n}=2+\left\{2 P_{u}(n-3 \mid k-3, z)+(n-4) P_{c}(n-3 \mid k-3, z)\right\} / P_{0}(k-3, z)$
and therefore (relations (7) and (A1.3, A1.4))

$$
\begin{equation*}
n m(n)=3 n+6+2(n-2)(2 z-n-7) /(z-1) . \tag{A3.5}
\end{equation*}
$$

If we fix $n$ and if we let $z \rightarrow \infty$, we end up with an unusual $m(n)=7-2 / n$, which increases when $n$ increases, with a distribution $P(n)\left(\mu_{2}=4\right)$ and with correlations $A_{k n}$ which verify all the required relations for $n, k \geqslant 4$ :

$$
\begin{equation*}
P(n)=(n-3) / 2^{(n-2)} \tag{A3.6}
\end{equation*}
$$

and
$A_{k n}=2+[4 n+4 k-32+2(n-4)(k-4)(n+k-10)] /\{(n-3)(k-3)\}$.
If we consider the cells with $n=z+1$ edges and if we let $z \rightarrow \infty$, we obtain from (A3.5) the expected value $m(\infty)=5$ instead of 7 given by the linear $n m(n)$ relation. It seems therefore unwise to let $z \rightarrow \infty$ in such tilings. The consistent set $P(n)$ and $A_{k n}$ given by (A3.6) and (A3.7) has nevertheless the merit to give rise to an Aboav-Weaire relation with $a=-1$.

## References

Abbruzzese G, Heckelmann I and Lücke K 1992 Acta Metall. Mater. 40 519-32
Aboav D A 1970 Metallography 3 383-90
_- 1980 Metallography 13 43-58
Babcock K L and Westervelt R M 1989 Phys. Rev. Lett. 63 175-8
Brakke K A 200,000,000 random Voronoi polygons Report Department of Mathematical Sciences Susquehanna University Selinsgrove PA 17870 USA no date ( $\sim 1985$ )
Carnal E and Mocellin A 1981 Acta Metall. 29 135-43
Conge H 1991 Invisible Works (Sarreguemines, France: Pierron)
Consul P C 1989 Generalized Poisson Distributions Properties and Applications (New York: Marcel Dekker) Statistics: textbooks and monographs vol 99
Delannay R, Le Caër G and Khatum M 1992a J. Phys. A: Math. Gen. 25 6193-210
Delannay R, Le Caër G and Sfeir A 1992b Proceedings of 12th Max-Entropy Workshop Paris July 1992 ed A Mohammad-Djafari and G Demoment (Dordrecht: Kluwer) in press

- 1993 in preparation

Fradkov V E, Shvindlerman L S and Udler D G 1987 Phil. Mag. Lett. 55 289-94
Fraser D P, Zuckermann M J and Mouritsen O G 1990 Phys. Rev. A 42 3186-95
Frost H J and Thompson C V 1987 Acta Metall. 35 529-40
Gervois A, Troadec J P and Lemaître J 1992 J. Phys. A: Math. Gen. 25 6169-77
Glazier I A 1989 PhD thesis University of Chicago IL, USA
Godrèche C, Kostov I and Yekutieli I 1992 Phys. Rev. Lett. 69 2674-7
Grünbaum B and Shephard GC 1987 Tilings and Patterns (New York: Freeman)
Lambert C J and Weaire D 1983 Phil. Mag. B 47 445-50
Le Caër G 1991a J. Phys. A: Math. Gen. 24 1307-17; 2677
_— 1991b J. Phys. A: Math. Gen. 24 4655-75

Lemaître J, Gervois A, Bideau D, Troadec J P and Ammi M 1992 C.R. Acad. Sci. Paris 315 35-8
Lemaître J, Gervois A, Troadec J P, Rivier N, Ammi M, Oger L and Bideau D 1993 Phil. Mag. B 67 347-62
Lewis F T 1931 The Anatomical Record 50 235-65
Mombach J C M, de Almeida R M C and Iglesias J R 1992 Phys. Rev. Lett., in press
Peshkin M A, Strandburg K J and Rivier N 1991 Phys. Rev. Lett. 67 1803-6
Righetti F, Liebling T M, Le Caër G and Mocellin A 1992 Materials Science Forum 94-6 791

- 1993 Acta Metall. Mater, to be submitted

Rivier N 1985 Phil. Mag. B 52 795-819
-_ 1986 Physica 23D 129-37

- 1993 Disorder and Granular Media eds D Bideau and A Hansen (Ansterdam: North-Holland) in press

Smith C S 1954 Scientific American 190 58-64
Stoyan D, Kendall W S and Mecke J 1987 Stochastic Geometry and its Applications (New York: Wiley)
Thompson D'A W 1917 On Growth and Form (Cambridge: Cambridge University Press)
Weaire D 1974 Metallography 7 157-60
Weaire D and Rivier N 1984 Contemp. Phys. 25 59-99
Yekutieli I 1992 PhD thesis, Saclay, France

