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MAXIMUM ENTROPY AND EQUATIONS OF STATE FOR RANDOM CELLULAR STRUCTURES*

N. Rivier
Materials Science Division
Argonne National Laboratory
Argonne, IL 60439

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MAXIMUM ENTROPY AND EQUATIONS OF STATE FOR RANDOM CELLULAR STRUCTURES

N. RIVIER*
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Argonne National Laboratory
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ABSTRACT. Random, space-filling cellular structures (biological tissues, metallurgical grain aggregates, foams, etc) are investigated. Maximum entropy inference under a few constraints yields structural equations of state, relating the size of cells to their topological shape. These relations are known empirically as Lewis's law in Botany, or Desch's relation in Metallurgy. Here, the functional form of the constraints is not known a priori, and one takes advantage of this arbitrariness to increase the entropy further. The resulting structural equations of state are independent of priors, they are measurable experimentally and constitute therefore a direct test for the applicability of MaxEnt inference (given that the structure is in statistical equilibrium, a fact which can be tested by another simple relation (Aboav's law)).

1. Introduction

We shall discuss the structure of soap froth, tissues, metallurgical grain mosaics, in short, of random space-filling cellular networks. These structures are at first glance all indistinguishable (apple, feather tissues look like soap froth, as do metallurgical ceramics), even though the local forces responsible for their architecture are very different (Weaire and Rivier 1984). These forces are therefore less relevant in molding the cellular structure than the inescapable, mathematical constraints of filling a topological space. This "universality", and the irrelevance of local, specific forces, are only possible if the structure is random. Why is it random? We shall see that randomness and space-filing imply remarkable (and observable) correlations in the cells. The main correlations are expressed in the structural equations of states (1) and (2), which are the focus of our discussion.

Maximum Entropy inference is the tool used. The present application of MaxEnt relies entirely on information expressible as constraints. It is independent of prior probabilities (which are here non-trivial measures as befits a continuous, geometrical problem) and constitutes therefore a direct test of the predicting power of MaxEnt methods.

Specifically, we will exploit the ability of MaxEnt to detect bias (in the colloquial sense). Bias manifests itself here through unexpected correlations between the size of cells and their topological shape (the number of sides). Roughly, larger cells have more sides. But a precise relation was discovered by Lewis (1928) in two-dimensional botanical tissues,

$$A_n = \alpha(n-n_0) \qquad (1)$$

and - a different correlation - by Desch (1919) in metallurgical grain mosaics,

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$$\Pi_n = \alpha'(n-n_o') \qquad (2)$$

Here A_n and Π_n denote the average area and perimeter (or radius) of n-sided cells.

Correlations (1) and (2) can only appear as constraints in MaxEnt formalism, since metallurgical and botanical mosaics, similar looking random space-filling cellular networks, should have the same a priori measures for the size and the shape of their cells. Then, the correlations are physical laws or unavoidable mathematical restrictions. Our aims are to understand their origin, and why grains differ from tissues.

Most of the results of this paper have already appeared in print. The guiding principle in explaining and establishing significant correlations in random cellular structure, especially their equation of state, has been Maximum Entropy. It is a privilege, in this forum, to return the compliment and use empirical structural correlations to illustrate the power and versatility of MaxEnt inference, as "a method of reasoning which ensures that no unconscious arbitrary assumptions have been introduced". (Jaynes 1957, p.16).

2. Elementary Topological Transformations and Detailed Balance

Tissues, froths, etc. are cellular graphs with interfaces (edges, and faces in 3D) meeting at vertices and forming polygons in 2D, polyhedra in 3D. Randomness has two, complementary manifestations: Interfaces do not have fixed length, but fluctuate, and the cells' number of sides n is a random variable. The second manifestation is a consequence of the first, as we shall see.

Fluctuations of its interfaces cause elementary, local topological transformations of the cellular network. In two dimensions (2D), there are only two types of transformations, neighbor exchange (T1) or cell disappearance (T2) (and its inverse). (Fig. 1). Cellular division or mitosis, the essential topological transformation in the growth of biological tissues, is an inverse T2, usually combined with a few T1.

These elementary topological transformations have two direct consequences. i) Only vertices of coordination 3 (4 in 3D) are structurally stable. A "Four Corner Boundary", the critical point of T1 transformation, is tipped either way by infinitesimal fluctuation. It occurs with negligible probability in random cellular structures. ii)

$$\langle n \rangle = 6 , \qquad (3)$$

for a 2D froth containing a very large number of cells. (A weaker relation holds in 3D) [Eq. (3) follows from Euler's relation, C-E+V = 1, between numbers of cells (C), edges (E) and vertices (V) of any large 2D (Euclidean) network, a topological conservation law (its left-hand side is conserved under elementary transformations), and from vertex coordination 3.]

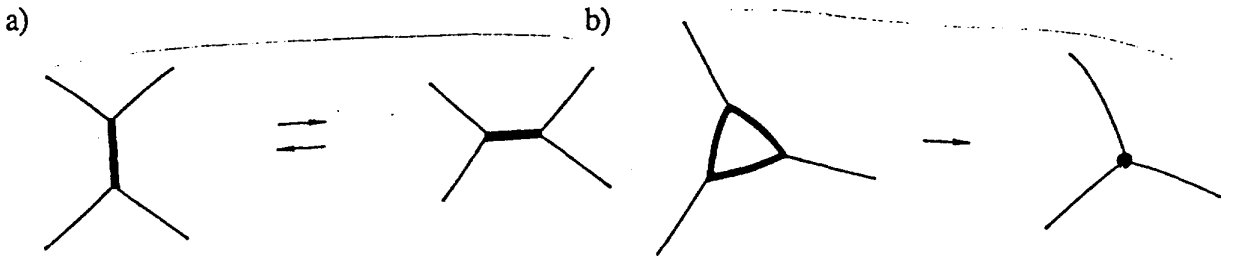

Figure 1. Elementary topological transformations in 2D cellular networks. a) Neighbor exchange (T1). b) Cell disappearance (T2).

Elementary topological transformations play the same role as collisions in kinetic theory of gases. They establish statistical equilibrium of the structure. [Indeed, concentrate on topological correlations m(n), where m is the average number of sides of any cell neighboring a n-sided cell. Unlike the constant <n>, m(n) is controlled by elementary topological transformations, which impose recursion relation between m(n) and m(n±1). Correlation m(n) is the solution of the same recursion relation for T1, T2, and their inverses. Elementary topological transformations can therefore occur independently, anywhere in the structure, and establish the observable correlation m(n), an empirical law due to Aboav (1971) which is universally obeyed by all known random cellular structures (cf. Weaire and Rivier (1984), Mombach *et al.* (1989))]. Aboav's relation indicates that the structure is in detailed balance under elementary topological transformations, a prerequisite for statistical equilibrium, whose characterization is our next step.

3. Statistical Equilibrium

Statistical crystallography (the description of cellular structures in statistical equilibrium) is based on the proposition that an assembly of an enormous number of cells will take up one of the most probable configurations subject to a few constraints like space-filling. The most probable configurations in the ensemble share the same equation of state, a relation between measurable, macroscopic parameters of the structure, and the same probability distribution function for the microscopic parameters. In kinetic theory of gases (Table 1), the equation of state is the ideal gas law (pV=NkT), and the distribution function Boltzmann's or Maxwell's distribution, with pressure p, temperature T and volume V as macroscopic parameters, and an atom's velocity or energy, its microscopic parameters {i}. The gas is in microscopic equilibrium as it satisfies detailed balance under collisions which are local, elementary transformations of the microscopic parameters. In liquids where atoms interact, a non-ideal equation of state like van der Waals's, reflecting their interaction, replaces the ideal gas law. Both equation of state and distribution function are obtained by maximizing the entropy, which takes the Gibbs form,

$$S = \sum_i p_i \ln p_i \,. \qquad (4)$$

The first triumph of MaxEnt formalism was to reformulate these physical results in information terms, ridding them of the their unnecessary overcoat of mechanical hypotheses like ergodicity (Jaynes 1957). Gibbs's entropy is identical to Shannon's measure of information, and MaxEnt yields the least biased or maximally non-committal distribution subject to available knowledge encoded in the constraints. But, if the distribution has been analyzed extensively in MaxEnt literature, the equation of state between macroscopic parameters has always been relegated as a somewhat trivial consequence, of interest to experimental physicists only. This is, emphatically, an oversight. While the distribution contains detailed information on the system, it also depends on the "priors" - the measure in phase (or event) space - information which cannot be encoded in constraints, and which is therefore not controllable by physical means. (Statistical mechanics, for which quantum mechanics (Nernst theorem) imposes that all cells in phase space are equally probable a priori is an exception.) By contrast, the equation of state gives a rougher account of the system (it relates macroscopic or average parameters), but it is independent of the priors, as we shall show, and only indicates how many, and which physical (chemical, mathematical or biological) constraints are relevant, a very desirable tool for the scientist: "If it can be shown that the class of phenomena predictable by maximum entropy inference differs in any way

from the class of experimentally reproducible phenomena, that fact would demonstrate the existence of new law of physics, not presently known" (Jaynes 1957, p.20). For "class of phenomena", read "equations of state", and you have the message and the content of this paper.

We shall see that froths, tissues, etc., are the least biased partitions of space, subject to a few, inevitable mathematical constraints pertaining to filling a topological space, and possibly, to an energy constraint. The surprise is that there is a particular way of filling topological space which increases the entropy, and therefore decreases the bias further, and this purely mathematical interplay between constraints is indeed reflected in botanical tissues: This is the content of their equation of state, Lewis's law (1). Additional constraints modify the structural equation of state (for example, from (1) into (2), see § 6), which becomes the simplest diagnostic tool for structural pathology.

4. Equation of State for Ideal Tissues. Lewis's Law

A cell in 2 dimensions is described by two microscopic parameters, its area A and the number n of its sides. We can marginalize the metric parameter A in the distribution function P (n,A), and concentrate on the shape distribution p_n

$$p_n = \int dA\, P(n,A) \tag{5}$$

The topological parameter n=3,4,...,N is an integer, so $\{p_n\}$ can be regarded as a vector in a N-2-dimensional space.

We want to find the most probable, or least biased distribution $\{p_n\}$, without going through the effort of computing the entropy (see Rivier (1985) for a complete solution). $\{p_n\}$ is subject to the inescapable constraints,

$$\begin{aligned} &\textstyle\sum_n p_n = 1\,, && \text{normalization} \\ &\textstyle\sum_n n\, p_n = 6\,, && \text{topology} \\ &\textstyle\sum_n A_n\, p_n = A_{tot}/C\,, && \text{space-filling}\,. \end{aligned} \tag{6}$$

Here, A_n is the average area of n-sided cells, $p_n A_n = \int dA\, A\, P(n,A) = p_n \int dA\, A\, P(A|n)$, A_{tot} is the total area available and C is the number of cells. The topological constraint is familiar (3). The constraints are linear in $\{p_n\}$, and occupy a space of dimension d (≤ 3).

The solution $\{p_n\}$ lives in a space of dimension

$$D = N - 2 - d\,, \tag{7}$$

the dimension of $\{p_n\}$ less that of constraint space. The larger the dimension D of the solution space, the more probable that solution, so that the most probable solution is obtained when the dimension d of the space of constraints is lowest. (Calculation of the entropy fully confines this argument of linear algebra (Rivier (1985), see also § 7).

Now, d will be minimal (=2) if one constraint can be made redundant, that is if the constraints (6) are linearly dependant. Using arbitrary coefficients λ_i, $0 = 1 - \lambda_1 n - \lambda_2 A_n = 1 - \lambda_1 6 - \lambda_2 (A_{tot}/C)$, one obtains,

$$A_n = (A_{tot}/C)\, \lambda\, [n-(6-1/\lambda)]\,, \tag{1'}$$

a relation between average sizes and shapes of cells, discovered empirically by Lewis (1928). It has slope $\langle A \rangle \lambda$ and intercept n_0,

$$(A_{tot}/C)\,\lambda = \langle A \rangle \lambda\,, \tag{8}$$

$$n_0 = 6\text{-}1/\lambda\,, \tag{9}$$

and implies that the average cell area $\langle A \rangle$ is equal to that of hexagons,

$$\langle A \rangle = A_{tot}/C = A_6\,. \tag{10}$$

Lewis's relation (1) was found originally in cucumber epidermis, human amnion (with an interesting comment (Lewis 1931) on the history of the sample in relation with its morphology) and pigmented epithelium of the retina; later in the epidermis of iris, begonia, and peas (Smoljaninov 1980, Fig 18-19), in iris stomata, axial fibroblasts and sections of the cerebellum of a mouse, cat and man (ibid, Fig. 26-27); also in onion, garlic, agave and anthurium (Mombach *et al.* 1989), and in the Voronoi cells of Poisson-distributed seeds ((Crain (1978); Two columns of his table are interchanged (Boots 1987)). All these tissues have intercept $n_0 \approx 1\text{-}2$, except for the Voronoi, the onion and the stomata $n_0 \approx 0$, and for the cerebella $n_0 \approx -2$. The intercept n_0 and slope of Lewis's law are given in term of the indeterminate multiplier λ (which serves indeed as a Lagrange multiplier in maximizing the entropy). We shall see in § 5 that λ is the time - it measures the ageing of the structure, at least for soap froth where a complete physical description of growth (von Neumann's law) is available. Thus, the larger the intercept n_0, the coarser and older (riper) is the structure. Fig. 2 reproduces Lewis's data (1931) on cucumber epidermis, and human amnion. If the average area A_n is linear in n, the range in areas of individual cells is large ($\approx 0.6\text{-}1\ A_n$).

Lewis's law is a structural equation of state, obtained because the tissue is free to adjust the arbitrary functional dependence of the constraint A_n in order to increase the entropy. The derivation is due to Rivier and Lissovski (1983). It raises several questions: 1) What is the parameter λ ? (Lagrange multipliers in physics are physical quantities, temperature, chemical potential, force of constraint, etc.). 2) Is Lewis's law universal ? Soap froths will be discussed presently, and I feel that they do obey Lewis's law despite their high n_0 (and λ). Metallurgical grain mosaics do <u>not</u>. They follow Desch's law (2) instead. Why ? (Note that A_n and Π_n are both averages, so that $A_n \neq \Pi_n^2$ in general.)

In soap froths (Glazier *et al.* 1989) as in the one photographic emulsion studied by Lewis (1931), the intercept $n_0 > 3$, so that the occurrence of a few three-sided cells badly spoils the linearity of Lewis's plot. However, these few cells are not statistically significant and the large, systematic departure from the linearity of Lewis's law for $n = 3$ is only a reflection of the impossibility of negative areas. Nevertheless, a definite conclusion on Lewis's law in soap froths must await statistical analysis of the data, which has yet to be made. In the froths, the average cell area A_{tot}/C equals from that of the hexagon, A_6, in agreement with Lewis's law (10). This is not the case in the emulsion.

5. Evolution, von Neumann's law and the meaning of λ

Soap froths, metallurgical grain mosaics and biological tissues evolve in time, through topological transformations induced by the fact that air diffuses out of small bubbles into the large ones, larger botanical cells are more likely to divide, and larger grains grow at the expense of smaller ones. The time scale for evolution is long enough for the froth to

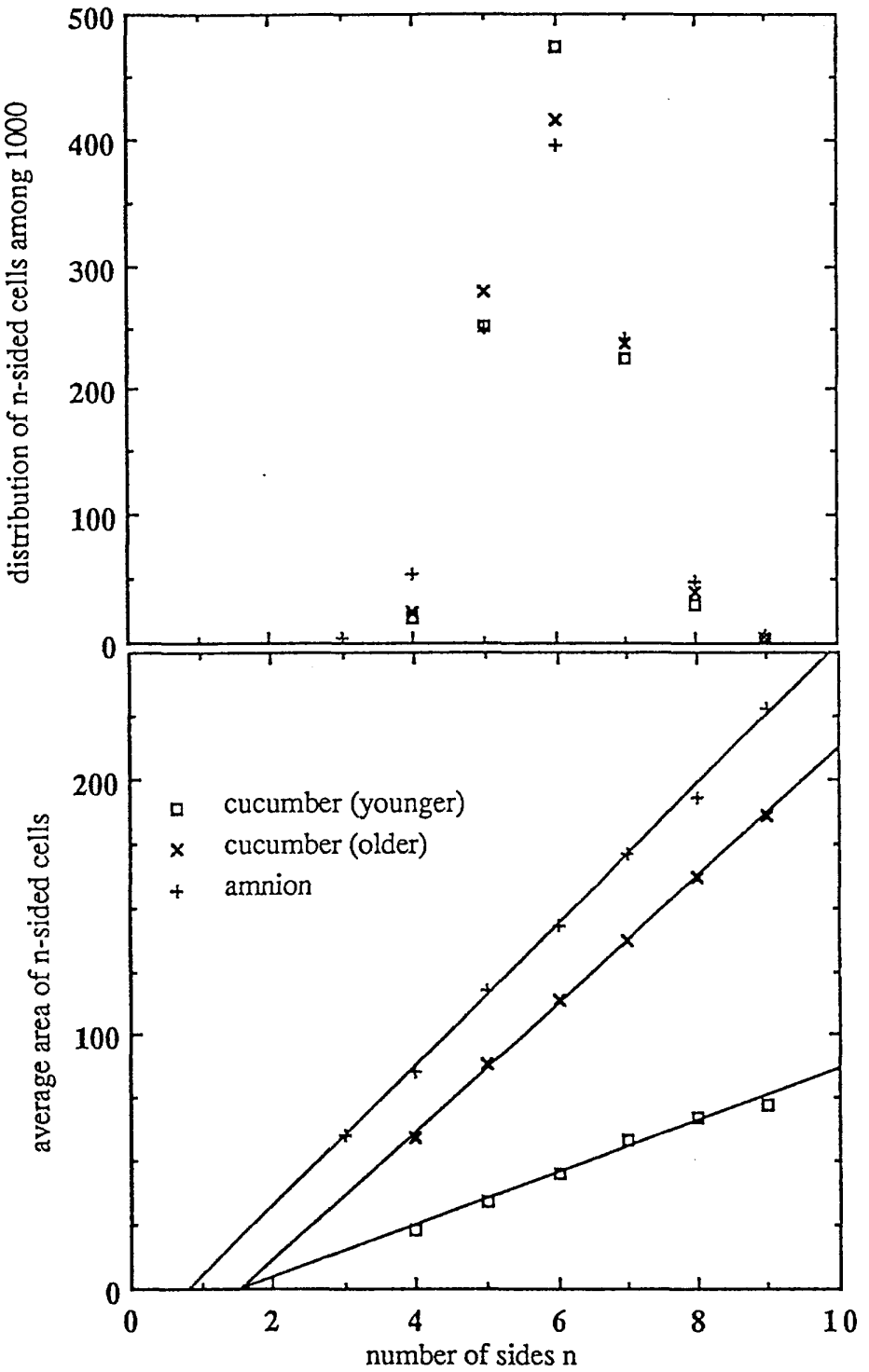

Figure 2. Lewis's law (1') and distribution of cell shape for cucumber and amnion. (Data from Lewis 1931). $\langle A \rangle = A_6$.

remain in statistical equilibrium and to satisfy its equation of state at all times. In thermodynamics, the evolution is then called quasistatic.

5.1 Coarsening. For an ideal tissue or froth, Lewis's law is obeyed at all times. The simplest case is a soap froth, where A_{tot} and C remain constant for a while (at least for young froths without triangular bubbles, so that no T2 transformations occur). Then, differentiation of Lewis's law (1') yields

$$(d/dt)A_n = (d/dt)\,[(A_{tot}/C)\,\lambda\,(n-6) + (A_{tot}/C)] = \gamma\,(n-6)\,, \qquad (11)$$

a relation obtained by von Neumann (1952) for 2D soap froths. Eq. (11) implies that the froth coarsens, a fact obvious to anyone washing the dishes. Von Neumann's derivation is a gem: A few, simple, physical laws conspire to produce a purely topological (and almost dimensionless) result (11). Any (not the average) pentagonal cell loses area at the same rate as any heptagon grows, at half the rate of any octogon, etc. The present derivation (Rivier 1983a) is slightly weaker because it involves averages, but like Lewis's or Desch's law, it can be generalized to 3 dimensions, and to all space-filling random structures in statistical equilibrium. [Von Neumann's independent derivation also shows that a froth need not obey Lewis's law to evolve according to (11) (as is the case for metallurgical aggregates)].

Von Neumann obtains $\gamma = 2\pi\sigma\delta/3 > 0$, where σ is the surface tension and δ the gas diffusivity across the interfaces. Here,

$$\gamma = (A_{tot}/C)\,(d\lambda/dt) > 0\,, \qquad (12)$$

hence,

$$\lambda = (C/A_{tot})\,\gamma\,t + cst\,, \qquad (13)$$

so the indeterminate multiplier λ is simply the time. It measures the ageing of the structure. The intercept of Lewis's law $n_0 = 6 - 1/\lambda$ (9) is therefore larger for older froths, which are also coarser and less uniform (the slope of Lewis's law, proportional to λ, is larger), a phenomenon known in metallurgical circles as Ostwald ripening.

If C does not remain constant (bubbles or grains disappear (T2)),

$$dA_n/dt = \gamma\,(n-n_1) \qquad (14)$$

$$n_1 = 6 - [(d/dt)\,(A_{tot}/C)]\,/\,\gamma < 6 \qquad (15)$$

$$\gamma = (d/dt)\,(\lambda A_{tot}/C) > 0\,, \qquad \lambda = (C/A_{tot})\int \gamma\,dt \qquad (16)$$

and the coarsening is qualitatively similar.

Why should metallurgical grains (whose evolution is driven by surface (grain boundary) tension) evolve like soap froths (which coarsen by diffusion of gas across interfaces from the smaller cells with high pressure into the larger ones) ? This is because the resultant of the surface tensions of three interfaces concurrent at a vertex is directed towards the cell with inner angle $< 2\pi/3$. Accordingly, hexagons with 6 angles equal to $2\pi/3$ are stationary, pentagons tend to shrink and heptagons grow. Recent simulation and modelisation of grain growth by Telley (1989) has made this result quantitative.

5.2 Botanical tissues. Steady state growth. In constrast, to froths or grains, biological tissues evolve by combination of growth [$(d/dt)\,A_{tot} > 0$] and cellular division [$(d/dt)\,C > 0$], while remaining structurally in a steady state. Cellular division (mitosis) is a combination of elementary topological transformations (inverse T2, together with one or several T1).

The steady state of vitally active botanical tissues has constant λ (which does not measure time any longer), thus constant intercept of Lewis's law, but increasing A_{tot} (continuous growth) and number of cells C (cell division). Strict steady state (topological invariance of the structure) corresponds to constant A_{tot}/C over times longer than the period of the mitotic cycle, and is achieved through interplay between continuous cellular growth and discrete mitoses. It is not quite realized in cucumber epidermis, in which $A_{tot}/C = A_6$ and Lewis's slope both increase with age, while the intercept $n_0 \approx 2$, thus λ, remains constant. (Fig. 2). Cucumber epithelia coarsen a little.

Topological steady state has been discussed elsewhere (Rivier 1988). It is interesting because it yields the average shape of cells just about to divide (n=7) and that of their two daughters (5.5), as well as the period of the mitotic cycle. An importance consequence of Lewis's law (already hinted at in the original paper of Lewis (1931)) is that if detailed balance holds for the topological variable n (and it does, as shown by Aboav's law), it automatically holds for the metric variable A, since

$$<A_n> = A_{<n>} . \tag{17}$$

Notably, the average growth rate of a cell is given by

$$d<A>/dt = \Sigma_n p_n (dA_n/dt) , \tag{18}$$

since

$$\Sigma_n A_n (dp_n/dt) = 0 \tag{19}$$

follows from topological and normalization constraints (6) and Lewis's law (1). Note that Eq. (19) does not imply topological steady state ($dp_n/dt = 0$).

The conclusion of the last two sections is a quotation lifted from Lewis (1931) paper: "Diese scheinbare Regellosigkeit sehr wohl geregelt ist" (Strasburger, 1866).

6. Metallurgical Aggregates, Desch's Law

In metallurgical aggregates, it is not the cell's area, but its perimeter Π_n (or radius) which is proportional to n, a relation (2) discovered also empirically and even earlier on by Desch (1919), and confirmed by computer simulations (Srolovitz *et al.* 1984).

MaxEnt inference, and the inevitability of all the constraints (6) used in deriving Lewis's law, immediately provide the explanation for this non-ideal behavior, namely the presence of an additional physical constraint. Clearly, there is energy concentrated in the interfaces or grain boundaries between cells, known as surface tension σ. Accordingly, the cell has an additional parameter, its perimeter Π, and the mosaic has an additional constraint,

$$\Sigma_n p_n \Pi_n = 2\sigma E/C \qquad \text{energy} , \tag{20}$$

besides the inevitable ones (6). Here $p_n = \int dA d\Pi\, P(A,\Pi,n)$ and $p_n\Pi_n = \int dA d\Pi\, \Pi\, P(A,\Pi,n)$. Maximization of entropy proceeds as in § 4. (The Lagrange multiplier enforcing the energy constraint (20) is the inverse temperature 1/kT, and we are on the solid grounds of classical thermodynamics.)

The functional dependence of Π_n, like that of A_n, is not imposed a priori. It can be adjusted to decrease the dimension of the space of constraints, and increase further the entropy. It turns out that there are only two alternatives (Rivier 1985), either A_n and n, or Π_n and n are linearly dependent, but not both. Moreover, the latter alternative has a slightly higher entropy S_{ME} than the former, but this fact does not rule out Lewis's law even in the presence of surface tension, because the two alternatives are disjoint in events space. At any rate, the presence of surface tension, in addition to the inevitable constraints (6), offers Desch's law,

$$\Pi_n = (2\sigma E/C)\,\lambda\,[n-(6-1/\lambda)]\,, \qquad <\Pi> = \Pi_6\,, \qquad (2')$$

as an alternative to Lewis's (1',10), as is indeed observed in metallurgical aggregates. Note that the slope, intercept and the average perimeter of Desch's law duplicate exactly the corresponding parameters of Lewis's law (8-10). The evolution of metallurgical mosaics (Ostwald ripening) is therefore expected to follow a von Neumann's type of law (11), but involving the cell's perimeter instead of its area. Again, λ is the time, and the mosaic coarsens,

$$(d/dt)\,(\lambda 2\sigma E/C) > 0 \qquad (21)$$

but there is no simple expression for this positive rate in terms of physical parameters, as we had in soap froths. Von Neumann's evolution for mosaics driven by surface tension has already been justified in § 5. Trigonometry shows that a hexagon in a mosaic, with 6 interfaces incident at $2\pi/3$ on its vertices, can swell or shrink freely without changing the interfacial length, i.e., at no cost in energy. The extent of this free breathing is only limited by topological transformations T1 and T2.

Von Neumann's proof of his law (11) refers to each cell individually, for which $A \propto \Pi^2$. Thus, $(d/dt)\Pi_n$, like $(d/dt)A_n$, is proportional to (n-6) if C remains constant, in agreement with evolution of Desch's law (2'). But the coefficient of proportionality $(1/2\Pi_n)$ depends on n.

Jaynes's scenario quoted in §3, has been performed in this section by metallurgical grains. The fact that the "new law of physics" (2) was actually known by a few metallurgists since 1919 should not detract from this demonstration of the predictive and diagnostic power of MaxEnt, and of the role in understanding and clarifying physical phenomena by identifying the relevant constraints. It also shows that there is fundamental physics besides Einstein's (at least in Germany in the late 1910's).

7. Maximum Entropy and the Number of Constraints

In deriving Lewis's (1) or Desch's (2) laws, we have adjusted the unknown functional form of the space-filling or energy constraint to increase the entropy. This absence of information on, or arbitrariness in the form of the energy or space-filling law, represented as an additional degree of freedom in the system, is measured by an increase of the entropy, as we shall now demonstrate.

Specifically, two constraints were made linearly dependent. Equivalently, the dimension of the space of constraints was decreased by one, or one constraint was made redundant. Let us see how this increases the entropy (Rivier 1983b).

Consider s constraints, labelled by $\alpha = 1...s$,

$$<c_\alpha> = \Sigma_n p_n c_{n\alpha} = X_\alpha = - (\partial/\partial\lambda_\alpha) \ln Z , \qquad (22)$$

imposed by the Lagrange multipliers λ_α, with

$$Z = \Sigma_n q_n \exp (- \Sigma_\alpha \lambda_\alpha c_{n\alpha}) = Z (\{\lambda_\alpha\}) . \qquad (23)$$

(The priors q_n, introduced for generality, are unimportant in our argument). The most probable, or maximum entropy S_{ME} subject to the constraints, and the distribution p_n are obtained by extremising the functional $-\Sigma_n p_n \ln p_n + \Sigma_\alpha \lambda_\alpha (\Sigma_n p_n c_{n\alpha})$,

$$S_{ME} = \ln Z + \Sigma_\alpha \lambda_\alpha X_\alpha = S_{ME}(\{X_\alpha\}) , \qquad (24)$$

which is a function of $\{X_\alpha\}$ only, since

$$\partial S_{ME}/\partial\lambda_\alpha = 0 \qquad (25)$$

is none other than the constraint equation (22). $S_{ME}(\{X_\alpha\})$ is therefore the Legendre transform of $\ln Z(\{\lambda_\alpha\})$, with

$$\partial S_{ME}/\partial X_\alpha = \lambda_\alpha , \qquad (26)$$

and

$$\partial^2 S_{ME}/(\partial X_\alpha)^2 = \partial\lambda_\alpha/\partial X_\alpha = (\partial X_\alpha/\partial\lambda_\alpha)^{-1} = -[<(c_\alpha - <c_\alpha>)^2>]^{-1} \leq 0 . \qquad (27)$$

The last equality comes from (22), and the mathematically obvious inequality, the positivity of specific heats, constitutes one of the earliest postulates of thermodynamics (Truesdell (1980), p. 16). The entropy is a convex function of its coordinates $\{X_\alpha\}$.

Consider now constraint ξ, say. The entropy S_{ME} is largest as a function of X_ξ when X_ξ is such that

$$\lambda_\xi = \partial S_{ME}/\partial X_\xi = 0 \qquad (28)$$

because of inequality (27). But the vanishing Lagrange multiplier $\lambda_\xi = 0$ makes the corresponding constraint ξ inoperative or redundant. This demonstration illustrates the discussion by Jaynes (1979) and Fougere (1988) of what counts as a degree of freedom in Chi^2 analysis.

8. Conclusions

The principles governing the structure of random cellular networks and their evolution (statistical crystallography) are those of statistical mechanics. Accordingly, the development of statistical crystallography is parallel to that of classical statistical thermodynamics (Table 1). Its centerpiece is the equation of state, obtained by maximizing the entropy. Here, the cellular network is free to use the unspecified form of the constraints to increase its entropy, and does so, yielding equations of states (1) and (2) which were already

known empirically. The ill-definition in the constraints is therefore a matter of physical indifference, a symmetry, rather than ignorance. A different equation of state would reveal the action of a new constraint, hitherto unidentified.

Slow evolution of the structure gives a physical meaning to the undetermined parameter in the equation of state. It is governed by an equation which is obtained almost automatically from the equation of state, but had been derived by von Neumann under specific physical assumptions. We are reminded of Jaynes' (1979, pp. 227, 232, and 236) comments as to how dynamics and ergodicity enter statistical mechanics: "Very efficiently".

TABLE 1. Methodology and equations of statistical thermodynamics and crystallography.

Thermodynamics	**Statistical**	**Crystallography**
	Random variables:	
(position), velocity $\Delta p\ \Delta x = h$		cell shape n, size A priors (geometrical measure)
	Detailed balance under:	
collisions		elementary transformations **-> Aboav law** (shape correlations)
	Statistical equilibrium (Maximum Entropy)	
	- equation of state (ideal)	
ideal gas law		**Lewis law**
	- equation of state (non-ideal)	
van der Waals, etc.		**Desch law**, etc.
	-most probable distributions	
Maxwell-Boltzmann		P(A,n) universality of cellular structures
	Slow evolution (quasistatic transformations)	
irreversible thermodynamics		**von Neumann law** (coarsening) or **steady state** (growth, mitosis)

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