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Shell Analysis and Effective Disorder in a 2D Froth

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The static and evolutionary properties of two-dimensional cellular structures, or froths, are discussed in the light of recent work on structuring of the froth into concentric shells. Of interest is the dual role of a topological dislocation ("defect") in an otherwise uniform froth, considered both as a source of disorder and also as a source generating a shell-structured froth. We present simulations on an initially uniform hexagonal froth. A defect is introduced by forcing either a T1 or T2 process in the stable structure, after which the froth is allowed to evolve according to von Neumann's law. In the first case, topological inclusions are found in the first few layers early in the evolution. In the second case, no inclusions appear over the entire evolutionary period. The growing disorder (as measured by the second moment of the side distribution, μ_2) is isotropic. For the special case of a T2-formed froth in a uniform network, the SSI structure is retained with $\mu_2 \neq 0$ only for the zeroth, first, and second layers. The ratio between topological perimeter and radius of the shells is close to 6, the value for a hexagonal froth.

KEY WORDS: 2D froth; shell-structure analysis; topological dislocation; shell-structured inflatability; topological inclusion; froth dynamics.

1. INTRODUCTION

Random, space-filling cellular structures occur commonly in nature, e.g., Weaire and Rivier (1984), Stavans (1993), Thiele *et al.* (1997) and references therein. The soap froth is the archetype for two-dimensional cellular patterns and is topologically stable, with three sides meeting at a vertex. The steady-state evolution of the froth has been characterised by laws describing the statistics of cell area, Lewis (1928), the growth rate of n-sided cells, von Neumann (1952), and scaling probabilities of cells, Stavans and Glazier (1989). Initially, correlation effects were assumed to be small and were considered to be almost completely described by the

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Aboav–Weaire law for nearest-neighbour correlation, Aboav (1970), Weaire (1974). Here, the average number of neighbours of an n-sided cell is given as $m(n) = (6 - a) + (6a + \mu_2)/n$, with μ_2, the second moment of the side distribution, $f(n)$, and a the Aboav–Weaire parameter. However, more detailed topological correlations have recently been derived, based on analysis of the froth as a system of concentric shells, which can be generated recursively, Aste *et al.* (1996a), Aste and Rivier (1997), Ohlenbusch *et al.* (1997). In particular, Dubertret *et al.* (1998) have shown, by maximum entropy arguments, that there is a linear topological correlation between two cells in a foam (or froth) in statistical equilibrium.

Shell-structure analysis is concerned with the definition of topological distance in a froth, where the distance j between any two cells, is the smallest number of edges crossed by paths connecting one to the other, Aste *et al.* (1996a). Any cell may be taken as the "germ" cell $j = 0$ and the froth may be viewed in terms of concentric layers or shells of equidistant ($j = 1, 2, \ldots$) cells, s.t. the jth layer of cells at distance j encloses layers $j - 1$, $j - 2, \ldots, 0$ and includes all cells which are themselves neighbours of at least one cell at distance $j + 1$. Any cell which does not obey this condition may be said to lie between layers $j - 1$ and j and represents a localised defect inclusion with respect to the froth "skeleton." Any froth, without defect inclusions, is called *shell-structured inflatable* (*SSI*), Aste *et al.* (1996a) and, in this case, shell-structure and skeleton coincide. Even though symmetry and periodicity information are absent, analysis of the shell-structure provides a powerful means of studying disordered froths.

By definition, no disorder is present in a 2-D uniform (hexagonal) froth, which is thus in mechanical equilibrium, (the state of minimum energy). A disordered froth typically undergoes topological changes, in order to achieve a state of statistical equilibrium, for which entropy is maximised, Dubertret *et al.* (1998). Any 2-D froth, not having minimum energy, will evolve according to von Neumann's Law, with an n-sided cell shrinking or expanding at a rate proportional to $n - 6$, von Neumann (1952). In the asymptotic steady state, topological properties are invariant, with μ_2 achieving a constant value and with the average cell area proportional to the square root of the time. Further, μ_2 provides an indicator of the level of disorder in the froth, which affects behaviour during the transient period, Ruskin and Feng (1997), together with the fraction of initial cells remaining. These are "survivors" of the evolution, i.e., cells which are present at a given time t_f and were also present at time t_i, $t_i < t_f$, Levitan *et al.* (1994), Levitan and Domany (1996). Clearly, any uniform hexagonal froth may have its mechanical equilibrium perturbed by the introduction of one or more topological dislocations, where each dislocation replaces one or more hexagonal cells. Of interest is the dual role of such a "defect," both as a disorder source and as a germ for the shell structure and the effect of this initial choice on the topological properties and froth evolution.

2. METHOD

In order to examine these questions, we have used the direct simulation approach of Weaire and Kermode (1983) to seed a uniform, (hexagonal), froth with localised disorder. A double dislocation or "defect" in this sense may be achieved by suppression of an edge in the original structure or by switching a side from one cell to its neighbour. Clearly, more than one operation of this kind may be used to randomly seed multiple dislocations, but we concentrate predominantly on the case for a single operation. Two types of topological double dislocations of the froth have been considered. The first is the pentagon–heptagon pairing, caused by forcing a T1 process, (neighbour switching) and where the central germ cell is considered to be the larger member. The second choice of germ cell is the eight-sided single cell, formed by a forced T2 process, (cell elimination). These are illustrated in Figs. 1 and 2 respectively. Clearly, any cell within the froth could be chosen as the centric germ cell to build up the shell structure. However, since most evolutionary properties are based on the contribution of "survivors" at different stages, it is more reasonable in a dynamic investigation to choose a survivor, rather than an eliminated cell to represent the original 0th centre. The choice of survivor cells, given here, is convenient for observing changes among shell layers during the froth evolution, although the theory applies equally to any other choice.

The froths generated are interesting, but rather special cases, in that the disorder is not uniform throughout the froth as a whole, but is highly

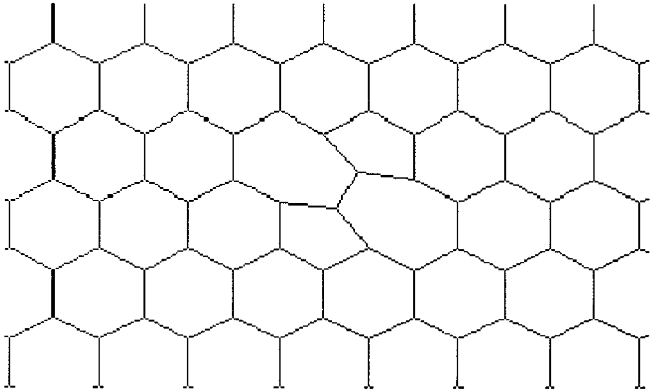

Fig. 1. SSI froth formed by T1 process.

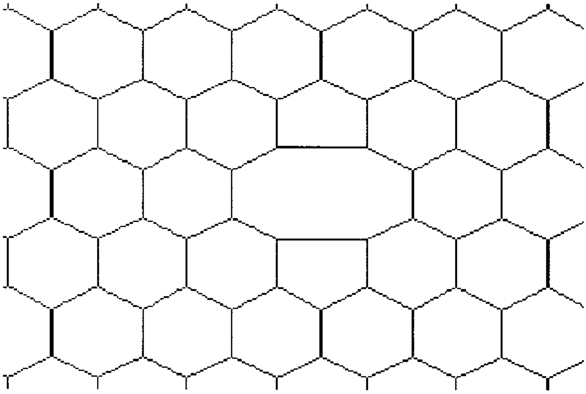

Fig. 2. SSI froth formed by T2 process.

localised and certainly not generic. The annulus of disorder is only a few cells in width and is reasonably typical of a normal froth. Outside this annulus, there is complete (hexagonal) order, with the froth in mechanical equilibrium. Inside the annulus, however, there is either a single large cell or a cluster of cells, larger than the others, with characteristics which asymptotically dominate the froth behaviour, Levitan (1994), Ruskin and Feng (1995). Departure from normal scaling for this region has been reported for finite systems and extensive simulations have been performed to investigate transience in relation to localised disorder, Jiang *et al.* (1995), Ruskin and Feng (1995), (1997) and Levitan and Domany (1996). It should be noted that these specialised structures contrast with a Voronoi froth, (Fig. 3), which is non-SSI, but also artificial, with high disorder levels and anisotropy of cells, compared to a typical froth, Boots (1982), Rivier (1985).

In the case of an SSI froth, the logistic map, Rivier and Aste (1996), used to give the number of cells in successive layers and to obtain average topological properties, can be written

$$K_{j+1} = s_j K_j - K_{j-1} \qquad (j \geqslant 1) \tag{1}$$

$$Q_j = 6 - K_{j+1} + K_j \tag{2}$$

where K_j is the total number of cells in the layer j, and $s_j = m_j - 4$ is a constant, (m_j is the average number of sides per cells in the layer j). The map starts with $K_0 = 1$ and $K_1 = n$, the no. of sides (or more generally neighbours) to the central cell. Equation (1) is due to Aste *et al.* (1996a) and Eq. (2) is a special case of the more general expression for topological charge, Q_j from the "Gauss" theorem, given by Rivier and Aste (1996).

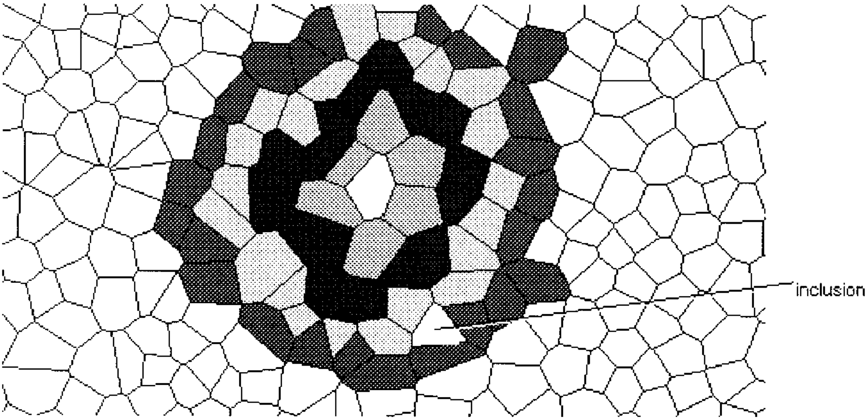

Fig. 3. Non-SSI froth formed by Voronoi network. Shades of grey indicate the different shell layers and topological inclusion is shown.

(Writing the K_j as V_j^+, V_j^- for outward and inward pointing vertices respectively on the closed line separating layers, one recovers the general form, which applies to any froth, whether SSI or not).

3. RESULTS

We report on the dynamics of the froth evolution in terms of the alternative method of analysing defect growth, linking this with the predictions of the shell map approach. Effective disorder is seeded by a single T1 or T2 topological dislocation, as described previously, and details of the simulation are as given in Ruskin and Feng (1995). In the present case, both seeded-disorder structures are initially SSI, according to the definitions given by Aste *et al.* (1996a). For the initial condition, it is obvious that the topological charge Q_j, (Eq. (2)), is constant from the second layer for both cases. Thus

$$K_{j+1} - K_j = K_j - K_{j-1} \qquad \text{for} \quad j > 1 \tag{3}$$

$$Q_j = 0 \qquad \text{for} \quad j > 1 \tag{4}$$

Equation (3) holds for both SSI and non-SSI froth and is the result of applying Eq. (1).

Following the very early period of evolution, the behaviour observed in the SSI froth formed by a T1 as opposed to a T2 process is markedly different. In particular, for the T1-formed froth, topological inclusion occurs very quickly in the first few layers, so that the structure becomes non-SSI for the remainder of the evolution, although the percentage of topological inclusions is small. However, for the T2-formed SSI froth, the basic structure remains SSI for the entire evolutionary period. No topological inclusions can be observed at any stage. Figures 4 and 5 show the froth evolution at a later stage (130 time steps) for T1 and T2-formed froth respectively, while the second moment, μ_2^*, (excluding the large cell(s)), reflects a quasi-scaling state in both cases, as noted by Ruskin and Feng (1996). Also, the number of cells in a layer increases linearly after the first few layers, so that for both germ cell choices, the relationship for K_j holds with

$$K_{j+1} = K_j + 6 \qquad \text{for} \quad j > p \tag{5}$$

where p depends on centre cell choice; $p = 3$ for large centre cell in T2-formed froth. (Linear growth of the number of cells has also been observed in recent experimental work, Szeto and Tam (1996)). Note that both correlation and self energies vanish for hexagonal cells.

Clearly, for initially SSI froths, μ_2 will change during the evolution. For most cases, inclusion will occur at some stage and the froth becomes

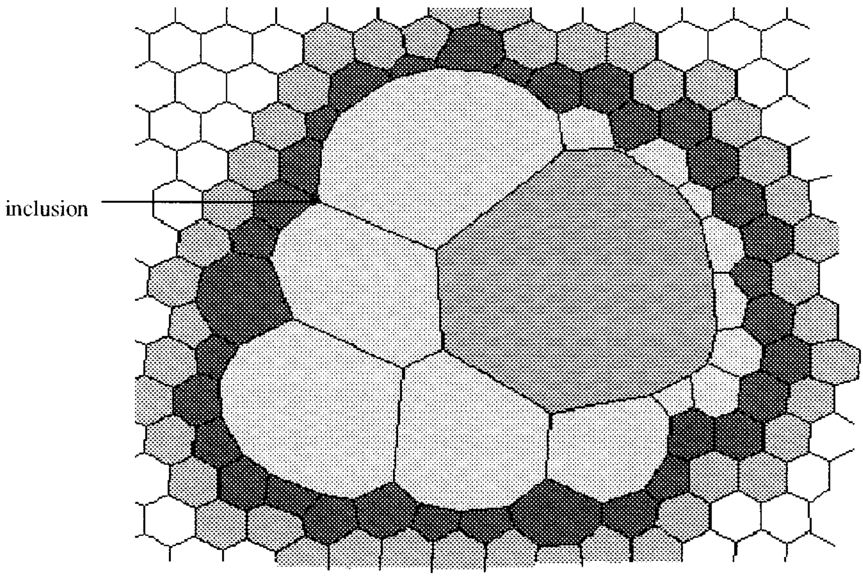

Fig. 4. The evolution of T1-formed non-SSI froth (after 130 time steps) with inclusion between layers $j = 1$ and $j = 2$. Shades of grey indicate the different shell layers.

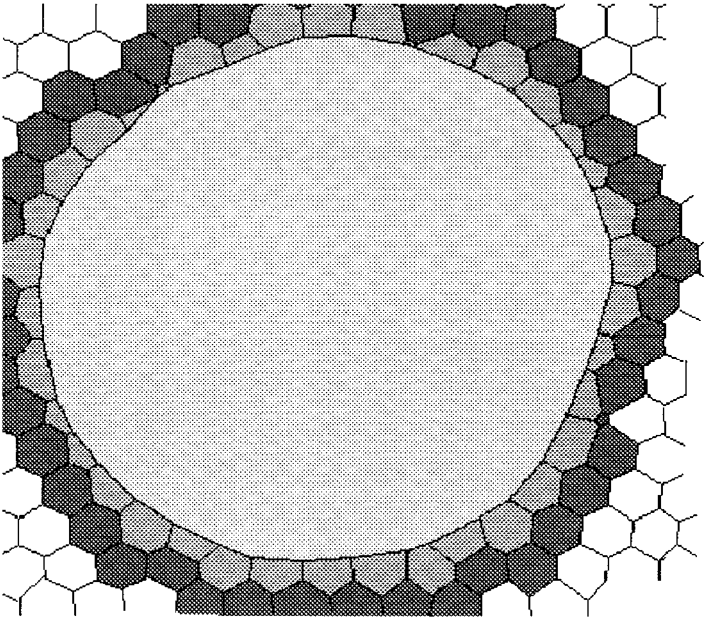

Fig. 5. The evolution of T2 formed SSI froth (after 130 time steps) without inclusion. Shades of grey again indicate the different shell layers. Small soon-to-disappear cells form part of the layer which immediately surrounds the large central cell (NW and NNE corners).

non-SSI. The only exception appears to be that of the single large cell, formed by a T2 process in a uniform froth. Here the SSI structure is retained with $\mu_2 \neq 0$ only for the zeroth, first and second layers. Thus, the original T2-formed disordered froth appears to be a valid case for a dynamic SSI froth. In the limit, as $t \to \infty$, the defect or central germ cell(s) consumes the froth and the number of its neighbours, (i.e. sides here), increases. At a given time t, the topological charge therefore consists of a large, negative contribution from the zeroth cell, a large number of smaller, mostly positive contributions from the narrow annulus and a zero-charge contribution from the outer hexagonal structure.

It seems intuitively clear that the perimeter should grow linearly with the topological radius and for a circular annulus the slope will be 2π, (although Aste *et al.* (1996b) measured a value of 9). In fact, disorder makes the slope much larger than 2π, in general, (see Aste (1997), Rivier (1997)). Including earlier layers for the SSI froth, we find the slope for the T2-formed example to be around 6.8–6.9, where the radius is based on the exscribed circle of the given layer. This is not too surprising, since the nature of the T2-formed defect means that near-circular layers are preserved in the froth evolution so that the ratio between topological perimeter and radius of the shells is close to the value for a hexagonal froth.

4. DISCUSSION

For initial correlation studies on these structures, Aste *et al.* (1996b) gave explicit expressions for K_j and Q_j for minimal correlation length and an approximate expression for the Aboav–Weaire law for higher shell numbers (ξ) expressed as

$$m_j K_j \approx 6K_j + (2-a)\,\mu_2 \qquad (j \geqslant \xi) \tag{6}$$

which is trivial for the second term on the right hand side $=0$. The authors suggested that, in the asymptotic limit (for j), a froth can only be free of defects if $\mu_2 = 0$ or $a = 2$, (although the latter is noted to be unrealistic). A more formal expression, relating the two-cell correlators, $A_1(k, n)$, for nearest-neighbours in natural foams to $n \cdot m(n)$, is given, Dubertret *et al.* (1998), as

$$n \cdot m(n) = \sum{}_k k f_k A_1(k, n) \tag{7}$$

where $A_1(k, n)$ is independent of the probability f_k that a k-cell exists and $f_k A_1(k, n)$ is the average number of k-cells, nearest neighbours to the n-germ cell. (The authors have generalised this for topological correlations in froths as a function of the layer distance j, with the $A_j(k, n)$ found to be linear in k and n).

In terms of correlation effects, the Aboav–Weaire law parameter, a, is of the order of 1 in most natural froths, (although not for T1-formed, or Voronoi Poisson froths for example, Peshkin *et al.* (1991), Boots (1982)). For the T2-formed froth, μ_2 does not, however, achieve a constant value, so that the approximate expression for the Aboav–Weaire law for second and further neighbours (Aste *et al.* (1996b)), does not apply. However, the total number of first neighbours is always known, which suggests that the more formal expressions relating two-cell correlations, Dubertret *et al.* (1998), may provide more insight on correlations between higher shell numbers. (We further comment that, although a special case, the T2-formed structure is of some interest experimentally,—see e.g., Abdelkader and Earnshaw (1997) for recent work).

The suggestion that $\mu_2 = 0$ is necessary for a defect-free froth is clearly incorrect, since we *do* see an SSI froth with $\mu_2 \neq 0$ in the studies described here. The anomaly appears to be due to the condition of $j > 2$, (quoted Aste *et al.* (1996b)), which assumes that μ_2 for the whole system is essentially that of μ_2, $(j>2)$. In fact, there are two possibilities for μ_2 when $j \leqslant 2$:

(i) if $\mu_2 = 0$ for $j = 0, 1, 2$, then, $\mu_2 = \mu_{2(j \leqslant 2)} + \mu_{2(j>2)} = \mu_{2(j>2)}$

(ii) if $\mu_2 \neq 0$ for $j = 0, 1, 2$, then, $\mu_2 = \mu_{2(j \leqslant 2)} + \mu_{2(j>2)} \neq \mu_{2(j>2)}$

The first condition relates to the mechanical equilibrium of the hexagonal network. The topological energy is always positive, with cells having correlation and self energies, Rivier (1997), and the former vanishing for the hexagonal, $\mu_2 = 0$, case only.

Based on structuring the froth into concentric shells, non-SSI froth with a small percentage of inclusions is expected to have similar properties to that of SSI froth. Considering the whole dynamic evolution, we expect statistical distributions to be very similar for both T1 and T2-formed froths, (Ruskin and Feng (1995), Jiang *et al.* (1995)). Nevertheless, these are aggregate measures and implications for the overall percentage of inclusions must be taken into account, Aste (1997). We also considered, therefore, *more than one* topological dislocation or introduction of a non-hexagonal cell formed by a T2 process, (i.e., multiple defects), and found that local defect inclusions will occur at some stage of the evolution. The SSI property is *not* retained indefinitely and the froth will become non-SSI at some point.

5. CONCLUSIONS

Direct simulation studies indicate that, for a T1-formed SSI froth, topological inclusion rapidly occurs in the first few layers so that the structure becomes non-SSI for the remainder of the evolution, although the percentage of local inclusions is small. For the T2-formed SSI froth, the basic structure remains SSI for the entire evolutionary period and is the only exception with $\mu_2 \neq 0$, only for the zeroth, first and second layers. This is the only exception that we can find to the general rule that topological inclusions will occur at some stage of the froth evolution.

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