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LETTER TO THE EDITOR

The evolution of a two-dimensional soap froth with a single defect

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Abstract. Using the direct simulation method of Weaire and Kermode, we consider the problem raised by Levitan of a 2-D froth with a single defect. We have found that, for a single defect in an ideal hexagonal network, the second moment, μ_2, of the distribution of the number of cell sides for the region of the defect does not tend to a constant as claimed by Levitan. Some reasons for the varying conclusions drawn by different authors about this problem are also discussed.

The soap froth as an ideal model of a cellular network has attracted considerable attention and has been studied theoretically and experimentally in recent years (see Weaire and Rivier (1984), Glazier *et al* (1987), Weaire and Lei (1990), Glazier and Weaire (1992), Herdtle and Aref (1992), etc). Interest has primarily focused on scaling properties obtained through the evolution of the froth with time. Long-term behaviour is characterized by system statistics such as the distribution, $f(n)$, of the number of cell sides and the second moment of this distribution, $\mu_2 = \sum(n-6)^2 f(n)$. There is considerable experimental, theoretical and computational evidence that μ_2 tends to a finite limit (approximately 1.4), which is characteristic of the asymptotic scaling state of the froth.

The initially transient behaviour of a relatively ordered froth has been interpreted in terms of the growth of individual topological defects. The study of this growth has been taken up by Levitan (1994), who considered the insertion of a single local topological defect into a froth of hexagonal cells. He used an approximation which is attractive in that it offers the potential to simulate larger, closer-to-asymptotic systems, but results obtained were in disagreement with previous tentative conclusions (Weaire in Blackman and Taguena 1991). We have, therefore, re-examined this problem by direct simulations which are more extensive than those previously undertaken.

Levitan's method first forces a T1 topological process (neighbour switching) to take place in a group of cells and follows this with a T2 process (cell elimination), for which the probabilities of a triangle, square and pentagon being formed are the same. In fact, the first T1 process gives rise to two five-sided cells and two seven-sided cells in the network (figure 1). Levitan used a mean-field theory to show that the topological distribution associated with a single defect approaches a fixed asymptotic form, with a high peak $f(6) \approx 0.6$. This implies that μ_2 attains a *different* and *stable* value in conflict with previous predictions.

Using the direct simulation approach of Weaire and Kermode (1983b, 1984) and subsequent work, we have implemented a 2-D dry froth with a single topological defect, based on a perfect hexagonal network to ensure correspondence with Levitan's original construction. The defect is based on a symmetrical arrangement of two pairs of pentagonal

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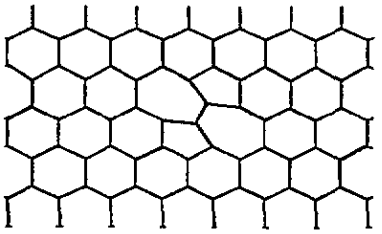

Figure 1. The defective 2-D froth network, corresponding to Levitan's method of inserting a single defect by forcing a T1 process in an ideal hexagonal froth.

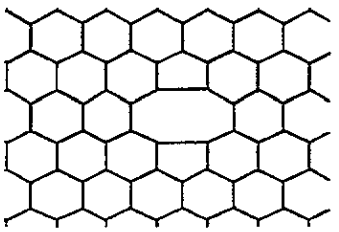

Figure 2. A defective 2-D froth network. The network keeps the hexagonal basis, and all the non-defective cells are of the same shape and size.

and heptagonal cells with minor discrepancies in the areas of the component cells and with all hexagonal cells surrounding the defect having the same area (figure 1). Additionally, we consider another type of topological defect, where the distortion is achieved by suppressing an edge in the original network giving an eight-sided cell with two symmetrical five-sided cells amongst its nearest neighbours (figure 2). We have also used an *ordered* Voronoi construction to create a third kind of defect (figure 3), in which the areas of the defect and its neighbouring cells have been adjusted as shown. Periodic boundary conditions are used but, for convenience, the defective cell is centrally placed in the network. Calculations are not pursued beyond the stage where the defect impacts on the boundary.

We have implemented the froth with single defects as shown (figures 1, 2, and 3), for systems of 100, 400 and 900 cells respectively. We give details of the results for a system of 400 cells as an example. Similar results are found for all system sizes used.

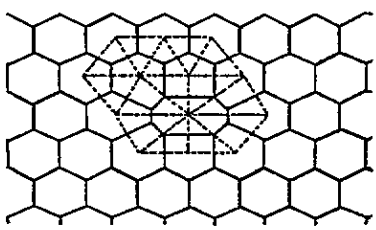

Figure 3. A defective 2-D froth network with an ordered Voronoi set-up. (Each vertex of an eight-sided cell and two five-sided cells is a centre of a circumscribed circle that corresponds to the Delauney tessellation.)

If we define an approximately circular 'front' of disturbance surrounding the large defective cell and including cells which have undergone a single topological change, the circular 'front' will include these (plus other cells which impinge on the circle in part, but which have not yet undergone change). Levitan (1994) similarly defines a 'cluster', which refers to the 'front' used in our simulations plus a boundary of hexagonal cells. The slight

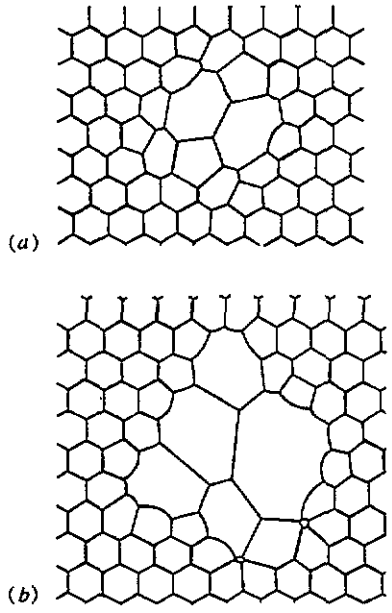

Figure 4. The evolution of a froth with a single defect in a hexagonal network with numbers of time steps of (*a*) 40 and (*b*) 100. (Initial structure figure 1.)

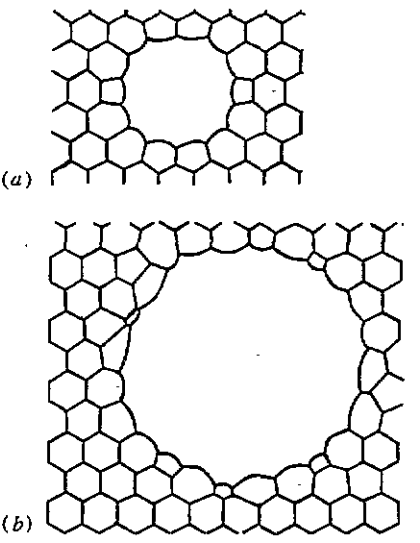

Figure 5. The evolution of a froth with a single defect in a hexagonal network with numbers of time steps of (*a*) 40 and (*b*) 100. (Initial structure figure 2.)

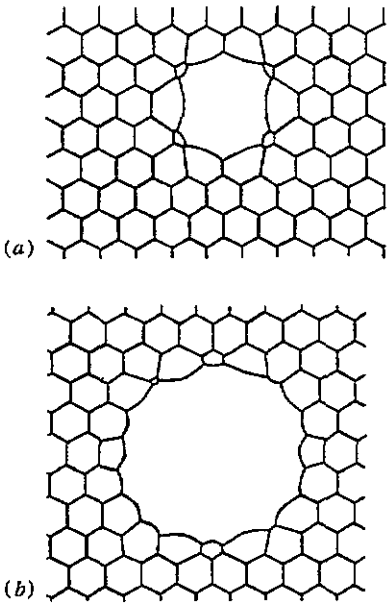

Figure 6. The evolution of a froth with a single defect in a hexagonal network with numbers of time steps of (*a*) 40 and (*b*) 100 respectively. (Initial structure figure 3.)

modification we have used does not affect the behaviour of μ_2 or the side distribution, but enables us to consider separately μ_2 *in the front.* Figures 4–6 show the evolution within the front at specific time steps for different initial defect types, corresponding to figures 1, 2, and 3 respectively. Here the number of time steps relates to the number of diffusion and equilibration processes which have taken place, with the evolution time, T, measured in units of $\langle A_0 \rangle / K$, where $\langle A_0 \rangle$ is the initial average area over all cells, and K is the constant

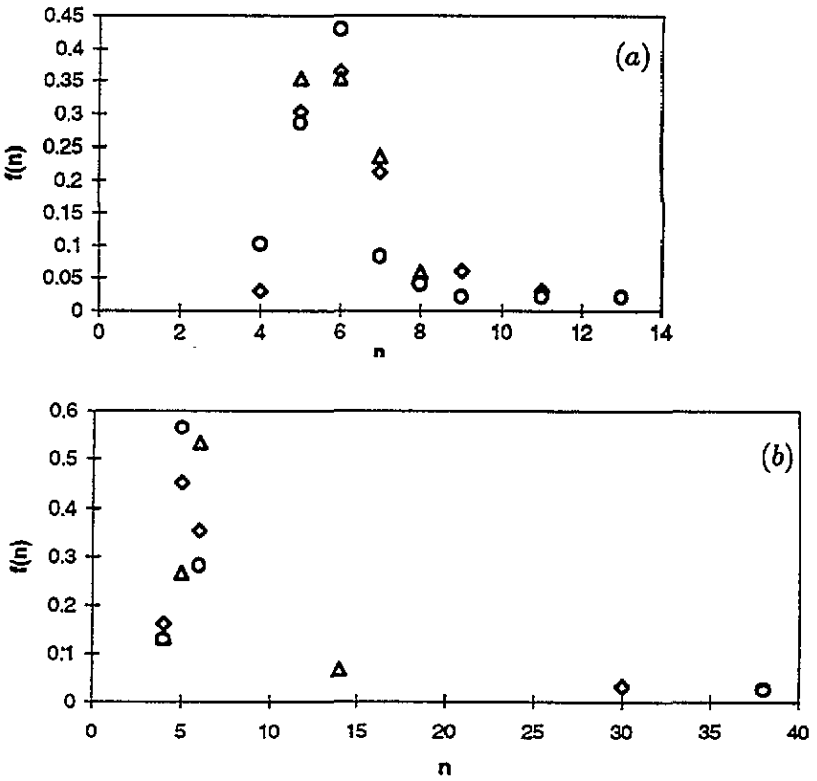

Figure 7. (*a*) and (*b*) show the topological distribution $f(n)$ in the *front* with numbers of time steps of 60 (△), 120 (◇), and 160 (○). (Initial set-up figures 1 and 2 respectively.)

in Von Neumann's law, and may be arbitrarily chosen (Kermode and Weaire 1990). We can see that the number of sides of the large defective cell increases with time, as does the perturbation front area of the disturbance. For the defect formed by edge suppression, starting from the ordered non-Voronoi network set-up (figure 2) and ordered Voronoi network (figure 3), we have observed very similar behaviour in the froth evolution (figures 5 and 6). We give detailed results for the initial structure shown in figures 1 and 2 as follows.

The topological distribution $f(n)$ *inside the front*, is shown in figures 7(*a*) and 7(*b*), at specific numbers of time steps for the different defect topologies (figures 1 and 2 respectively). We find that there tends to be a peak at $n = 5$ in the front as evolution time increases, as opposed to the overall network of a normal froth which has a peak with $n = 5$ and $n = 6$ (Herdtle and Aref 1992). However, the distribution $f(n)$ is now, of course, markedly right-skewed. These features are not extraordinary as movement of the front results in continual incrementation of the number of sides of the large defective cell.

From our results, the second moment, μ_2, continues to change with time *without* reaching a fixed limit. Figures 8(*a*) and 8(*b*) show how the second moment, μ_2, in the *overall* network changes versus time, T (for initial set-ups in figures 1 and 2). The range of T includes about 200 diffusion and equilibration processes in our simulation. Topological and diffusive adjustments are made sequentially within each time step and considerable details of the evolution may be observed. Fluctuations in the value of μ_2 around the underlying trend can be explained directly in terms of the T1 and T2 processes, with a high μ_2 corresponding to the defect surrounded by a number of three- or four-sided cells, and

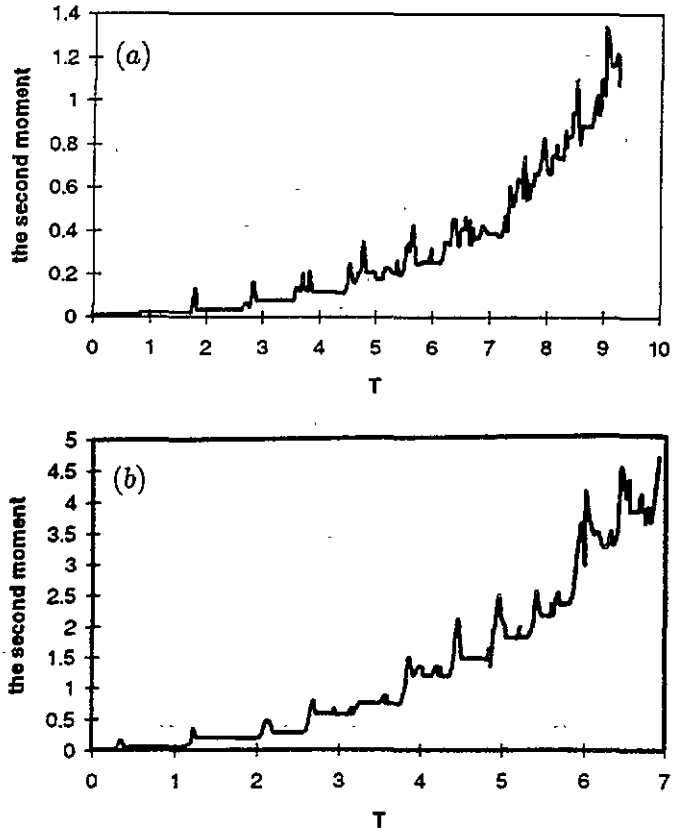

Figure 8. (*a*) and (*b*) show μ_2 in the *overall* network versus time T for a froth of 400 cells. (Initial set-up figures 1 and 2 respectively.)

a sudden decrease in μ_2 associated with the disappearance of one of these cells. During growth in the area of the defect, μ_2 keeps a relatively stable value until the next T1 occurs. Clearly, as more cells are involved in the evolution and the number of sides of the defect increases, the value of μ_2 *overall* changes more rapidly and is dominated by the contribution of the defective cell. Over the whole range of T, $\mu_2 \sim T^{\beta}$ appears to describe the observed behaviour, with $\beta > 1$. However, few changes take place initially, relative to the evolution as a whole, and for the upper range of T, μ_2 versus T is roughly linear, although it is not clear that a true asymptote is attained.

For a simple theoretical model of a large defect with N sides surrounded by N small cells, newly converted side lengths of the small cells will be characteristic of the whole network, i.e. $N \sim A(d)^{0.5}$, with $A(d)$ the area of the defect. Then, in the asymptotic limit, Von Neumann's law becomes $\mathrm{d}A(d)/\mathrm{d}t = kA(d)^{0.5}$, i.e. $A(d) \sim T^2$. Similarly, *in the front*, the topological distribution will be dominated by the defect, so $\mu_2(d) \sim N^2$ with $N \sim T$, i.e. $\mu_2(d) \sim T^2$. Furthermore, the defect gradually involves more and more cells in the overall network, so asymptotically the exponents for the front and the overall network should be the same. From our simulations, we find *for the defect* that $A(d)$ increases with T at the expense of other cells distorted by topological changes. If we define the increased area $\Delta A(d) = A(d) - A(d)_0$, where $A(d)_0$ is the original area of the defect, for the defect formed by edge suppression (figures 2 and 3), we obtain roughly $\Delta A(d) \sim T^2$ after the initial period of evolution, with the radius of the rough perturbation circle, $r \sim T$

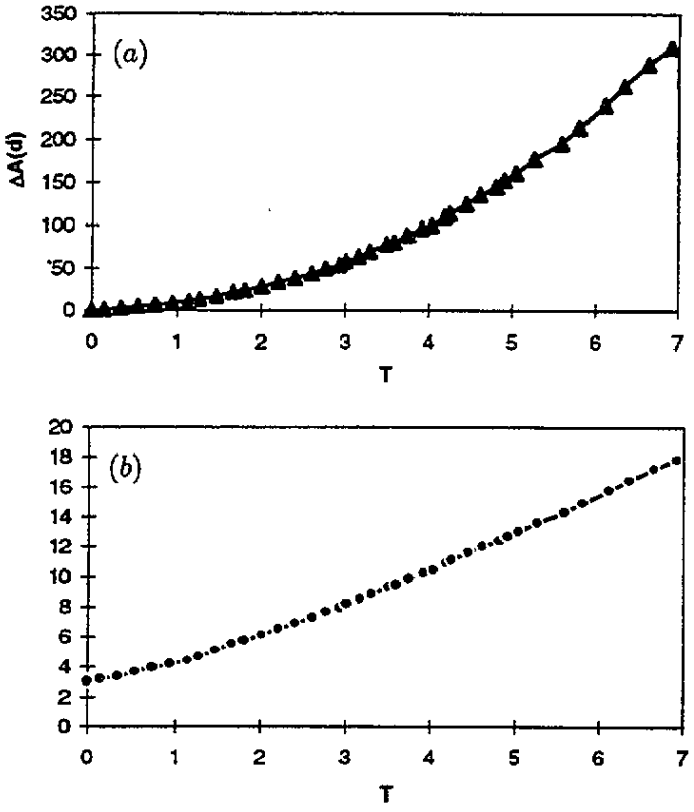

Figure 9. (*a*) The increase in defective area $\Delta A(d)$ versus time, T. (*b*) The radius r versus time, T, for a froth of 400 cells. (Initial structure figure 2.)

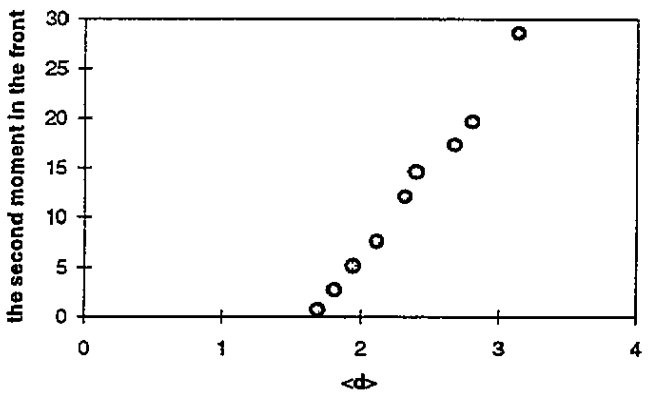

Figure 10. $\mu_2(d)$ in the *front* versus the average intercept, $\langle d \rangle$. (Initial structure figure 2.)

approximately; figures 9(*a*) and 9(*b*) illustrate for the set-up of figure 2. Furthermore, we find that $\mu_2(d)$ changes roughly *linearly* with the average intercept, $\langle d \rangle$, where $\langle d \rangle$ equals the square root of the average cell area in the front (figure 10).

It seems clear that the behaviour of a froth with a single defect in a uniform hexagonal network does *not* lead to a normal scaling state as found for the non-defective froth by

numerical simulation (and as predicted by theory). We find that $f(n)$ in the front tends to develop a long tail extending to large values of n and with a peak at $n = 5$. This is in agreement with Aboav (1980), who also quoted $\alpha = 2$ for the area growth exponent. However, the suggestion that μ_2 *overall* varies linearly with time (see the comment by Weaire and Kermode (1983a) on Aboav's work) is not wholly supported by our findings and is in conflict with the predictions of the simple model. It is only with hindsight that it has been realized that Aboav was dealing with a transient system with defects, characterized by different values of the growth exponents. Our own results are probably not in the asymptotic region since the maximum number of sides achieved by any defect is $N = 44$ (for the set-up in figure 2). Nevertheless, they are supported by recent work by Glazier (1995). We also find that there is some similarity between the behaviour of our system and that of Levitan (1994), but we do *not* agree with a *fixed* form for $f(n)$ as obtained by Levitan. The value of μ_2 (whether for the front or for the overall network) does not reach a steady state after initial fluctuations at this system size, unlike normal froth evolution.

Our results for the behaviour of the front are in agreement with the original experimental work of Aboav (1980), and recent simulations of Glazier (1995), indicating that a different scaling relation applies there. Regardless of the defect type and initial configuration, there are some grounds for support of the suggested system behaviour put forward by Levitan (1994), but the overall results are in conflict with his predictions for the quantities characterizing the long-term evolution.

We should like to thank Professor Denis Weaire for several interesting discussions and for introducing us to the froth problem.

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