Relation between volume, number of faces and three-dimensional growth laws in coarsening cellular patterns

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ABSTRACT

The recently established linear growth law for three-dimensional diffusive coarsening shows zero average growth for grains with 15·8 faces, while the average number of faces per grain in the pattern is 13·7 ± 0·1. In the better-known two-dimensional case, grains with six sides (the average number) show zero growth. We show that the three-dimensional zero growth value is a consequence only of the linear form of the law and the cubic dependence of average area per grain on the number of faces.

Until recently, most detailed studies of grain growth have concentrated on two-dimensional rather than three-dimensional cellular patterns, because the former are much easier to observe experimentally and faster to simulate (Glazier 1989, Glazier and Weaire 1992). Early three-dimensional Potts model simulations, although suggestive, did not measure the growth properties of individual grains (Anderson, Grest and Srolovitz 1985, 1989, Grest, Srolovitz and Anderson 1988).

Recent light-scattering experiments measuring the averaged growth rate in three-dimensional soap froths have stimulated renewed interest in the details of three-dimensional evolution (Durian, Weitz and Pine 1990, 1991a, b).

Von Neumann's (1952) analytically derived linear relationship between a cell's number of sides and its growth rate is a cornerstone of the theory of coarsening of two-dimensional cellular patterns:

$$\frac{\mathrm{d}a_n}{\mathrm{d}t} = \kappa(n - n_0), \tag{1}$$

where κ is a diffusion constant, a_n is the area of an n-sided grain and n_0 is a constant. The existence of such a simple relation, which is true exactly for each individual grain, greatly assisted the development of both exact and mean-field theory models of two-dimensional grain growth.

However, no one has succeeded in deriving a similar analytical growth law in three dimensions. Recently Glazier (1993), analysing the coarsening behaviour of the three-dimensional Potts model, concluded that a similar but weaker law holds for ensembles of bubbles in three dimensions. That result is

$$v^{-1/3}\left[\frac{\mathrm{d}v}{\mathrm{d}t}\right] = \kappa(f - f_0), \tag{2}$$

where κ is a diffusion constant, f is the number of faces of a grain, f_0 is a constant, v is the volume of a grain having f faces. However, this equation only holds *on average*. The growth rate of any individual grain need not depend on its number of faces; for example some 16-faced grains grow, while others shrink. Sire (1993) has addressed the reasons why only an averaged growth law holds in three dimensions.

In von Neumann's law, n_0 is the average number of sides per cell, which Euler's theorem fixes at exactly six. While a naive argument by analogy with von Neumann's law in two dimensions might suggest that $f_0 = 13.7$, the average number of faces of the grains in the pattern in the scaling state, Glazier found a value of $f_0 = 15.8 \pm 0.1$.

In this letter we explain the observed value of the constant f_0. Glazier (1993) had noted the apparent discrepancy but not addressed it. Sire (1993), while providing reasonable mean-field theory arguments for the linearity of eqn. (2), took both the value of f_0 and the relationship between faces and volume as parameters.

We show now that the difference between f_0 and $\langle f \rangle$ is a simple consequence of the face–volume relationship and the factor $v^{-1/3}$ in eqn. (2). We begin by noting that the total volume of the pattern is constant, that is

$$\left\langle \frac{dv}{dt} \right\rangle = 0, \tag{3}$$

where $\langle \ \rangle$ denotes averages over the entire pattern at a fixed time. Substituting from eqn. (2) yields

$$\langle v^{1/3}(f - f_0) \rangle = 0. \tag{4}$$

Phenomenologically, the average volume $\langle v_f \rangle$ of an f-faced grain depends on the cube of its number of faces (Anderson *et al.* 1985, 1989, Grest *et al.* 1988). Our estimate based on two $200 \times 200 \times 200$ third-nearest-neighbour zero-temperature Potts model runs (for details see Glazier (1993)) between 5000 and 50 000 Monte Carlo steps (MCSs) yields an exponent of 3.07 ± 0.17, compatible with an exponent of exactly three. We chose the starting time of 5000 MCSs to eliminate the most obvious transients while preserving reasonable statistics. However, the true equilibration time to reach a scaling state is substantially longer than 5000 MCSs. The typical value of the exponent increases slightly during the runs as the number of grains decreases (from about 3.05 at 5000 MCSs to about 3.15 at 50 000 MCSs) but always remains within one standard deviation of three. At any fixed time, the actual fits are good for small f but usually poor for large f. We therefore take (on the assumption of a scaling state)

$$v_f^{1/3} \propto f. \tag{5}$$

Substituting into eqn. (4) and averaging first over cells with fixed numbers of faces reduce eqn. (3) to

$$\langle f(f - f_0) \rangle = 0 \tag{6}$$

if we approximate the average of the cube root by the cube root of the average. Hence,

$$f_0 = \frac{\langle f^2 \rangle}{\langle f \rangle} = \langle f \rangle \left(1 + \frac{(f - \langle f \rangle)^2}{\langle f \rangle^2} \right) = \langle f \rangle \left(1 + \frac{\mu_2}{\langle f \rangle^2} \right). \tag{7}$$

Given the two empirically derived relations expressed by eqns. (2) and (5), eqn. (7) is exact.

Our Potts model runs show some long-term transients in their values for both $\langle f \rangle$ and μ_2. Between 5000 and 50 000 MCSs, $\langle f \rangle = 13\cdot7 \pm 0\cdot1$ (typical values decreasing from around 13·8 at 5000 MCSs to around 13·6 at 50 000 MCSs) and $\mu_2 = 29 \pm 6$ (typical values increasing from 22 to 35 over the same time interval). However, the values of f_0 are much more stable, since the changes in $\langle f \rangle$ compensate those in μ_2. Typical values for f_0 are 15·5 at 5000 MCSs and 16·1 at 50 000 MCSs. Averaging eqn. (7) over the entire time period yields

$$f_0 = 15\cdot8 \pm 0\cdot4, \tag{8}$$

substantially different from $\langle f \rangle = 13\cdot7 \pm 0\cdot1$ and agreeing precisely with the result of Glazier (1993).

The success of this derivation reinforces our confidence in Glazier's claim that the averaged growth rate in the Potts model is a linear function of the number of faces. The relation given in eqn. (7), or a similar generalization, should apply to any other coarsening system in which similar connections between growth rate, v and f apply.

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