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The average rate of growth of individual cells in a cellular structure: effect of the number of topological elements

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Equations are derived for the average rate of growth or shrinkage of individual cells in two- and three-dimensional cellular structures, when the driving forces for displacement are the excess free energies associated with faces and edges. Curvature effects are neglected. It is shown that in three-dimensional structures, such as polycrystals, cells (grains) with fourteen or more faces tend to grow while those with thirteen or less faces tend to shrink, the rate of growth/shrinkage increasing as the number of faces increases/decreases. In two-dimensional structures, the threshold between growth and shrinkage is for cells with six sides. The specific behaviour of particular cells can be predicted from a simple geometrical construction and can be quite different from the behaviour of the average cell with the same number of edges.

1. Introduction

In a recent publication [1] a thermodynamic analysis of grain growth was developed and the driving forces responsible for it, which are associated with the excess free energy of grain boundaries (faces) and triple lines (edges), were identified. It is convenient to adopt the following nomenclature: each force is identified by the topological element on which it acts and by the topological element whose free energy is responsible for the force. For example, an edge–face force acts on an edge and is due to the excess free energy of a face connected to the edge (grain boundary free energy). Face–face and edge–edge forces are due to the curvature of the corresponding topological elements. In addition to these there are, in 3D-structures, vertex–edge forces. In 2D-structures, the forces are edge–edge and vertex– edge. It will be assumed that no other driving forces (e.g. strain energy) are responsible for grain growth.

The forces produce displacements of the topological elements with a velocity that can be taken as proportional to the forces (constant mobility). Topological changes occur during movement of the topological elements which, in particular, lead to cell elimination and therefore to cell growth. The evolution of a given structure can be followed in a computer if the specific surface and line free energies are known and if the mobilities of vertices, edges and faces are also known. Computer simulations along this line for 2D-structures, acted by vertex–edge forces, are under progress and the results will be published elsewhere [2].

In this paper the average rate of growth (or shrinkage) of individual cells in relation to the number of topological elements they possess (i.e. the number of faces in 3D and the number of edges in 2D) will be considered. It will be shown that in 2D-structures, cells with less than 6 sides tend to shrink while those with more than 6 sides grow; in 3D-structures the threshold "shrinkage–growth" is for a number of faces between 13 and 14. Equations will be derived for the rate of growth of average individual cells.

The fact that cells with more than 6 sides tend to grow and those with less than 6 tend to shrink is generally accepted but is based on an argument due to Smith [3]. He assumed that the edges in a 2D-network meet at 120° so as to equilibrate the vertex–edge forces at each vertex. The edges must then in general be curved, in such a way that the resulting edge–edge forces produce growth of cells with more than 6 sides and shrinkage of those with less than 6 sides. Actual networks do not in general have 120° degrees in vertices, so that vertex–edge forces are also relevant to growth and cannot be ignored. Besides, the required curvature cannot occur in a (connected) network where, for example, a cell with 7 sides may be adjacent to one with 8 sides.

On the other hand, it was shown by Von Neumman [4] (see also [5]) that in a 2D soap froth, evolving by diffusion of the (incompressible) gas in the bubbles, the rate of change of the area A_n of cells with n sides is proportional to $(n - 6)$

$$\frac{\mathrm{d}A_n}{\mathrm{d}t} = k(n - 6) \quad (1)$$

In the situations that will be analysed here, growth occurs for other reasons and it is not expected, *a priori*, that Equation 1 still holds in those situations.

The growth of 3D-structures has received much less attention. The result that we obtain for these structures is perhaps expected, considering that natural structures such as polycrystals usually have an average number of faces per cell, $\bar{F}$, close to 13 to 14, (e.g. [6]), although cellular structures of the topological type of polycrystals may occur for any $\bar{F}$ between 8 and ∞ [7].

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In the following analysis it will be assumed that face–face and edge–edge forces are not relevant in grain growth. This simplification is necessary because the consideration of curvature would considerably complicate the analysis and no simple correlation could be obtained between growth rate and the number of edges or faces. The assumption can be justified if the mobilities of faces in 3D and of edges in 2D, are much larger than the mobilities of the other elements, so that they remain straight during growth. We consider in turn 2D- and 3D-structures.

2. Growth in two-dimensional structures

The forces responsible for growth, under the simplification enunciated above, are vertex–edge forces exclusively. These are indicated in Fig. 1a for a cell with 5 sides. Each vertex is acted by three line tensions, $\bar{\varepsilon}$, along the edges connected at that vertex. Isotropy and homogeneity will be assumed so that ε is the same for all edges.

For any n (number of edges), the cells are in general of different sizes, are not regular polygons and the outer edges connected at each vertex of the cell are not regularly oriented. We make the simplifying assumption, justified in the Appendix, that the average behaviour of n-sided cells can be described in terms of a single, regular polygonal cell with n edges and with the outer edges symmetrically distributed, i.e. in the direction of the bisectors of the angles of the polygon (Fig. 1b). This polygonal cell can be inscribed in a circle of radius R, which will be taken as a characteristic linear dimension of the cell. Since the internal angle in a regular n-gon is

$$\alpha_n = \pi\left(1 - \frac{2}{n}\right) \qquad (2)$$

the resultant driving force, F_v, on each vertex acts radially and has the value (positive if acting outwards)

$$F_v = \varepsilon\left(1 - 2\cos\frac{\alpha_n}{2}\right) \qquad (3)$$

For a constant mobility, M_v, of the vertices, the rate of change of R (velocity of the vertex) is

$$\frac{dR}{dt} = \varepsilon M_v\left(1 - 2\cos\frac{\alpha_n}{2}\right) \qquad (4)$$

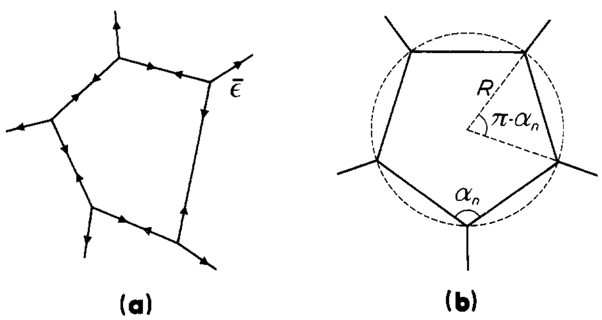

Figure 1 A pentagonal cell in a 2D-network with three edges connected at each vertex. Driving forces, $\bar{\varepsilon}$, along the edges act on each vertex. The growth behaviour of irregular cells with 5 sides [such as (a)] is described in terms of an "average" regular cell with the outer edges directed along the bisectors of the regular polygon, as shown in (b).

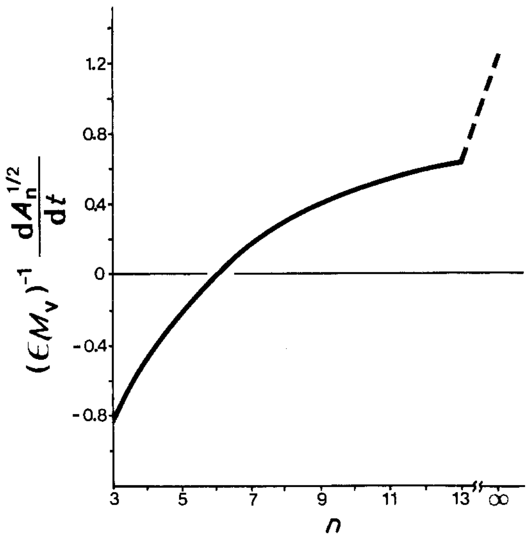

Figure 2 Rate of change of $A_n^{1/2}$ for polygonal cells with n sides in a 2D-network acted by vertex–edge forces.

Simple geometry gives for the area of a n-gon of dimension R

$$A_n = \frac{R^2}{2} n \sin\alpha_n \qquad (5)$$

Combining Equations 4 and 5 yields

$$\frac{dA_n^{1/2}}{dt} = \varepsilon M_v\left(\frac{n}{2}\sin\alpha_n\right)^{1/2}\left(1 - 2\cos\frac{\alpha_n}{2}\right) \qquad (6)$$

with α_n given by Equation 2. The rate of growth is positive for $n > 6$, negative for $n < 6$ and zero for $n = 6$. Fig. 2 shows the plot of $(\varepsilon M_v)^{-1}(dA_n^{1/2}/dt)$ as a function of n. It tends to $(\pi/2)^{1/2}$ as $n \to \infty$.

In order to compare with Equation 1 for the soap froth we obtain from Equation 6

$$\frac{dA_n}{dt} = 2A_n^{1/2}\frac{dA_n^{1/2}}{dt} = \varepsilon M_v R n \sin\alpha_n \times\left(1 - 2\cos\frac{\alpha_n}{2}\right) \qquad (7)$$

with α_n given by Equation 2. Equation 7 shows that the rate of growth, measured by the rate of increase of area, is proportional to the linear dimension R and does not vary linearly with n, as in Equation 1. The similarity between Equations 1 and 7 is only qualitative, in that they both predict a threshold at $n = 6$ between growth and shrinkage. It should also be noted that Equation 1 is valid for any cell with n-sides, while Equation 7 defines the behaviour of a regular cell with n-sides and symmetrical outer edges.

3. Growth in three-dimensional structures

Assuming that faces remain planar (and edges straight) the forces responsible for growth are edge–face and vertex–edge forces (Fig. 3). We consider an "average" polyhedron with F faces and assume that the faces are identical polygons with n sides, n being related to F through (e.g. [6])

$$n = 6 - \frac{12}{F} \qquad (8)$$

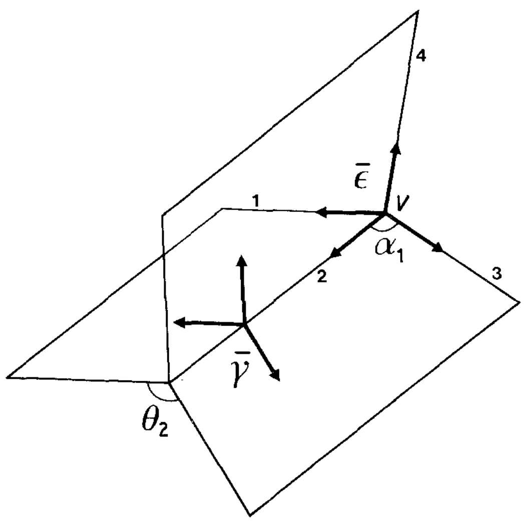

Figure 3 One vertex (V) and the four connected edges (1 to 4) in a 3D-network, with indication of the forces $\bar{\varepsilon}$ acting on the vertex and the forces $\bar{\gamma}$ acting on edge 2.

For fixed F, there is not a fixed value for the sum of the angles between faces connected at edges or between edges connected at vertices. For example, if we truncate a regular cube at a vertex to obtain a triangular face in a polyhedron of 7 faces, we can vary the orientation of the plane of the cut and in this way vary the individual and average angles between faces and between edges. In the "average" polyhedron these angles are well defined and can be calculated as follows.

Let α_1, α_2 and α_3 be the angles between pairs of edges of a polyhedron meeting at a vertex (α_1 is the angle between edges 2 and 3, etc.; Fig. 3). It is easily shown that the angle θ_1 between the faces of the polyhedron connected at edge 1 is given by

$$\cos\theta_1 = \frac{\cos\alpha_1 - \cos\alpha_2\cos\alpha_3}{\sin\alpha_2\sin\alpha_3} \tag{9}$$

and similarly for θ_2 and θ_3. In the average F-edron all faces are regular n-gons, with n given by Equation 8. Therefore

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_n = \pi\left(1 - \frac{2}{n}\right) = \left(\frac{F-3}{F-2}\right)\left(\frac{2\pi}{3}\right) \tag{10}$$

and the angle θ between two faces connected at an edge in the F-edron is, from Equation 9,

$$\cos\theta = \frac{\cos\alpha_n}{1 + \cos\alpha_n} \tag{11}$$

If the outer faces and edges are assumed to be symmetrically connected to the reference polyhedron, then the outward driving force edge–face at each edge is

$$F_e = \gamma\left(1 - 2\cos\frac{\theta}{2}\right) \tag{12}$$

where γ is the face excess free energy per unit area (surface tension); and the outward force edge–vertex at each vertex is

$$F_v = \varepsilon(1 - 3\cos\beta) \tag{13}$$

where ε is the edge tension and β is the angle between an edge of the polyhedron and the direction of the outer edge connected at the same vertex. This angle can be related to α_n, the angle between two edges of the polyhedron at a vertex

$$2\cos\alpha_n = 3\cos^2\beta - 1 \tag{14}$$

Therefore the outward driving force on a vertex can be written as

$$F_v = \varepsilon[1 - (3)^{1/3}(1 + 2\cos\alpha_n)^{1/2}] \tag{15}$$

Both F_e and F_v change sign when F changes. This happens, in both cases, for $\cos\alpha_n = -1/3$, leading to $F = 13.3973$ ($\bar{n} = 5.1043$). This value of F was indicated by Smith [6] as defining an "equilibrium" polyhedron.

It is fairly easy to obtain equations for the rate of change of the dimensions of the average cell with F faces under these driving forces. We consider first growth governed by the driving forces F_e only (Fig. 3). Denoting by D the distance of an edge to the centroid of the regular F-edron we may write

$$\frac{dD}{dt} = M_e F_e \tag{16}$$

The polyhedron can be divided into F regular pyramids with n lateral faces, D being the height of these faces. The solid angle at the vertex of the pyramid is $4\pi/F$, which corresponds to an average angle ϕ between the axis of the pyramid and the straight lines through the vertex of the pyramid and lying on lateral faces; ϕ is given by

$$\cos\phi = 1 - \frac{2}{F} \tag{17}$$

From this, we obtain for the volume of the polyhedron

$$V = 8D^3\left(1 - \frac{2}{F}\right)^2\left(1 - \frac{1}{F}\right)\tan\frac{\pi}{n} \tag{18}$$

which gives an error of 5% when applied to the (regular) cube ($D = a/(2)^{1/2}$, a-cube edge). The quantity $V^{1/3}/D$ given by Equation 18 is a slowly varying function of F (between 0.909 and 0.832 for F between 4 and ∞). Therefore for grain growth controlled by edge–face forces we have

$$\frac{dV^{1/3}}{dt} = 2M_e\gamma\left\{\left[\left(1 - \frac{2}{F}\right)^2\left(1 - \frac{1}{F}\right)\tan\frac{\pi}{n}\right]^{1/3} \times\left[1 - 2\left(\frac{1 + 2\cos\alpha_n}{2 + 2\cos\alpha_n}\right)^{1/2}\right]\right\} \tag{19}$$

with n given by Equation 8 and α_n by Equation 10. The plot of $dV^{1/3}/dt$ is shown in Fig. 4, curve E.

A similar analysis can be undertaken for vertex controlled cell growth (Fig. 3b). In this case the characteristic dimension, D', is the distance of the vertices of the cell to its centroid. The relation between V and D' is

$$V = 8D'^3\left(1 - \frac{2}{F}\right)^2\left(1 - \frac{1}{F}\right)\tan\frac{\pi}{n} \times\left[1 + \sin^2\phi\tan^2\frac{\alpha_n}{2}\right]^{-3/2} \tag{20}$$

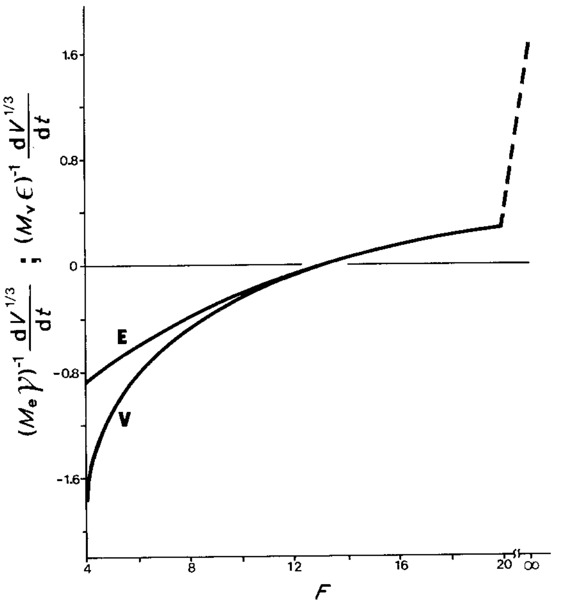

Figure 4 Rate of change of $V^{1/3}$ for polyhedral cells with F faces in a 3D-network acted by edge–face forces (curve E) and vertex–edge forces (curve V).

with ϕ given by Equation 17. Equation 20 gives an error of 1% when applied to the (regular) cube ($D' = a3^{1/2}/2$). The plot of $dV^{1/3}/dt$ for vertex controlled growth is also shown in Fig. 4, curve V. It is obtained by combining Equations 15 and 20 with

$$dD'/dt = M_v F_v \quad (21)$$

The more general case of driving forces acting both on edges and vertices is difficult to analyse because compatibility conditions on the displacements of the two types of topological elements have to be introduced. Besides, the global kinetics would depend on the ratio $M_e\gamma/M_v\varepsilon$, a quantity that is difficult to estimate.

4. Concluding remarks

Equations were obtained for the average rate of growth of individual cells in a cellular structure, the growth being governed by the excess free energy associated with the various topological elements. The equations were based on a somewhat loose averaging procedure. Nevertheless the results give some insight on the kinetics of growth and explain the tendency of polycrystals to have average values, $\bar{F}$, of F close to 14. It should be noted, however, that several models [8] of solidification of a liquid into a polycrystal lead to values of $\bar{F}$ close to 14, and this could also explain the experimentally observed values of $\bar{F}$.

Cells with more than 14 faces tend to grow and those with less than 14 faces tend to shrink. In two-dimensions, the critical value of the number of sides is 6. These results explain the experimental observation that large cells tend to have many sides and vice versa. It is also expected that the more regular cells (more uniform distribution of angles and more equiaxial) are those that change at a slower rate (see Appendix).

The growth of a cellular structure involves topological changes that were not considered in the present discussion. The actual cells are not regular and during growth may change their topology through a neighbour switching operation or through the removal of the simpler cells (those with $n = 3$ in 2D and $F = 4$ in 3D). The equations obtained give the average rate of change of dimensions of cells in classes with a given n or F while they remain within the same class. The complications that result from the topological changes are difficult to analyse and can only be characterized in a complete computer simulation of the process of growth. This procedure can also be used to check the accuracy of the equations derived in the present paper.

Appendix

Evolution of polygonal cells acted by vertex forces

The displacement of a vertex in a cell of given geometry depends on the orientation of the outer edge connected at the vertex. The final position of the vertex can be determined graphically by considering three equal vectors along the edges and finding their resultant. It is easy to show that as the orientation of the outer edge is varied (within the outer angle defined by the two other edges), the locus of the final positions of the vertex is in an arc of circle, between the two edges of the cell, and with its centre C on the bisector of the two edges, as shown in Fig. 5. The displacement of the vertex in time Δt is $M_v \Delta t |\Sigma_i \bar{\varepsilon}_i|$ where $\bar{\varepsilon}_i$ are the line tensions with $|\bar{\varepsilon}_i| = \varepsilon$. Using this construction it is straightforward to find the permissible shapes that result from the forces on the vertices of a given cell. Fig. 6 shows the locii of the final positions of the vertices of two hexagonal cells. Using this procedure we arrived at the following conclusions, as regards the effect of the orientation of the outer edges and the effect of the internal angles and shape of the cell, on the rate $dA_n^{1/2}/dt$.

(a) For any n, it is always possible to choose the orientation of the outer edges so as to induce a decrease in area. It is enough to take the edges as in the example of Fig. 6a (dashed lines).

(b) In regular polygons, the largest final area is obtained for orientations of the outer edges in the directions of the bisectors. This is not in general true for non-regular polygons.

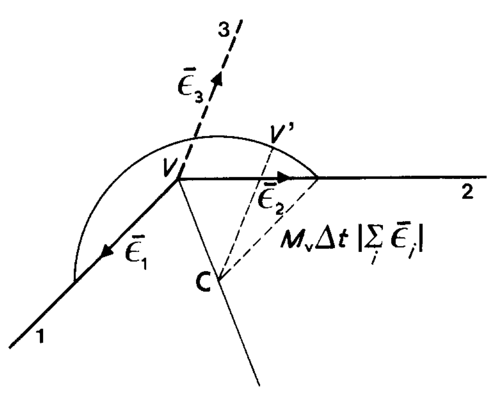

Figure 5 The edges 1, 2 belong to a cell and meet at vertex V; edge 3 is the outer edge connected at V. The arc of circle is the locus of the (finite) displacements of V acted by the (equal) line tensions $\bar{\varepsilon}_1$, $\bar{\varepsilon}_2$ and $\bar{\varepsilon}_3$ in the direction of the outer edge. The centre C of the circle is in the bisector of $\bar{\varepsilon}_1$ and $\bar{\varepsilon}_2$. Position V' corresponds to the orientation of the outer edge indicated by the dashed line.

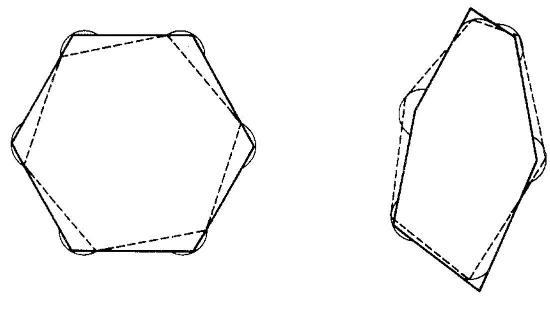

Figure 6 The locus of the final positions of the vertices of an hexagonal cell: (a) for a regular hexagon, showing a "final" cell of smaller area; (b) for an irregular hexagon, showing a "final" cell of larger area.

(c) When the perimeter of a polygon increases at constant internal angles, constant area, and constant orientation of the outer edges, the absolute value of $\mathrm{d}A_n^{1/2}/\mathrm{d}t$ increases. Equiaxility therefore decreases the absolute value of the rate of change of $A_n^{1/2}$.

(d) Large internal angles tend to originate an increase in area (or a smaller decrease), particularly if the associated edges are long. For example, it is possible to have an increase in the area of the irregular hexagon shown in Fig. 6b by the dashed lines.

(e) If an n-cell contains an edge much shorter than the others, the corresponding $\mathrm{d}A_n^{1/2}/\mathrm{d}t$ approaches that of a cell with $(n - 1)$ sides which is obtained by extending the edges adjacent to the short edge. This confirms the conclusion that equiaxiality decreases the absolute value of the rate of change of linear dimensions.

It follows that the rate $\mathrm{d}A_n^{1/2}/\mathrm{d}t$ can be larger or smaller than that for the regular polygon with the same n. The average value of $\mathrm{d}A_n^{1/2}/\mathrm{d}t$ for each n could in principle be calculated by considering all cells with n sides and all orientations of the outer edges. Even if the problem could be solved, it would probably not correspond to the average cell behaviour in a network because there are topological restrictions on the distribution of angles in a network related to the fact that some cell adjacencies are forbidden [1]. A correct determination of the average rate of change of dimensions should take these topological limitations into account; the problem is complex, which justifies the simplified averaging procedure used.

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